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Theoretical Investigation
of the Lowest Five Ionization Potentials
of Uranium

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FOREWORD

An exploratory experimental and theoretical investigation of gaseous nuclear rocket technology is being conducted by the United Aircraft Corporation Research Laboratories under Contract NASw-847 with the joint AEC-NASA Space Nuclear Propulsion Office. The Technical Supervisor of the Contract for NASA is Captain W. A. Yingling (USAF). Results of the investigation conducted during the period between September 15, 1964 and September 15, 1965 are described in the following eleven reports (including the present report) which comprise the required third Interim Summary Technical Report under the Contract:

1. McFarlin, D. J.: Experimental Investigation of the Effect of Peripheral Wall Injection Technique on Turbulence in an Air Vortex Tube. UAC Research Laboratories Report D-910091-5, September 1965. (Unclassified)
2. Johnson, B. V.: Analytical Study of Propellant Flow Requirements for Reducing Heat Transfer to the End Walls of Vortex-Stabilized Gaseous Nuclear Rocket Engines (U). UAC Research Laboratories Report D-910091-6, September 1965. (report classified Confidential)
3. Travers, A.: Experimental Investigation of Peripheral Wall Injection Techniques in a Water Vortex Tube. UAC Research Laboratories Report D-910091-7, September 1965. (Unclassified)
4. Johnson, B. V., and A. Travers: Analytical and Experimental Investigation of Flow Control in a Vortex Tube by End-Wall Suction and Injection (U). UAC Research Laboratories Report D-910091-8, September 1965. (report classified Confidential)
5. Mensing, A. E., and J. S. Kendall: Experimental Investigation of the Effect of Heavy-to-Light-Gas Density Ratio on Two-Component Vortex Tube Containment Characteristics (U). UAC Research Laboratories Report D-910091-9, September 1965. (report classified Confidential)
6. Krascella, N. L.: Theoretical Investigation of the Opacity of Heavy-Atom Gases. UAC Research Laboratories Report D-910092-4, September 1965. (Unclassified)
7. Kesten, A. S., and R. B. Kinney: Theoretical Effect of Changes in Constituent Opacities on Radiant Heat Transfer in a Vortex-Stabilized Gaseous Nuclear Rocket (U). UAC Research Laboratories Report D-910092-5, September 1965. (report classified Confidential)

8. Marteney, P. J., N. L. Krascella, and W. G. Burwell: Experimental Refractive Indices and Theoretical Small-Particle Spectral Properties of Selected Metals. UAC Research Laboratories Report D-910092-6, September 1965. (Unclassified)
9. Williamson, H. A., H. H. Michels, and S. B. Schneiderman: Theoretical Investigation of the Lowest Five Ionization Potentials of Uranium. UAC Research Laboratories Report D-910099-2, September 1965. (Unclassified)(present report)
10. McLafferty, G. H., H. H. Michels, T. S. Latham, and R. Roback: Analytical Study of Hydrogen Turbopump Cycles for Advanced Nuclear Rockets. UAC Research Laboratories Report D-910093-19, September 1965. (Unclassified)
11. McLafferty, G. H.: Analytical Study of the Performance Characteristics of Vortex-Stabilized Gaseous Nuclear Rocket Engines (U). UAC Research Laboratories Report D-910093-20, September 1965. (report classified Confidential)

Report D-910099-2

Theoretical Investigation of the Lowest Five Ionization
Potentials of Uranium

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Theoretical Investigation of the Lowest Five Ionization

Potentials of Uranium

SUMMARY

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Ionization potentials were calculated for uranium and its first four positive ions using approximate quantum mechanical methods. A range of values was obtained for each ionization potential, with the individual values depending upon the approximations entering into the calculations. The final suggested values are: U(I) - 6.11 e.v.; U(II) - 17.5 e.v.; U(III) - 37.5 e.v.; U(IV) - 61 e.v.; U(V) - 118 e.v.

Ionization potentials for U(I) through U(III), differing only slightly from these final suggested values, were employed in an evaluation of the following properties of equilibrium mixtures of hydrogen and uranium: species concentration, coefficients of viscosity and diffusion, and effective Schmidt number. The calculations were performed at pressures of 100, 500, and 1000 atm., temperatures of 20,000 K, 60,000 K, and 100,000 K, and fuel partial pressure fractions of 0.09, 0.1, 0.233, 0.367, 0.5, 0.633, 0.767, and 0.9. The results of these calculations indicate that the uranium ions of lower valency play an important role in the determination of the properties of the mixture up to temperatures higher than had been indicated in preceding studies, thereby raising significantly both the mixture viscosity and effective hydrogen-uranium binary diffusivity at temperatures below about 60,000 K. Since the changes in these two quantities are in the same direction, however, changes in the effective Schmidt number are small.

Bentley

INTRODUCTION

In studies of gaseous nuclear reactor concepts, the ionization potentials of neutral uranium and several of its positive ions are required in order to evaluate the transport properties, optical opacity, and radiant heat transfer characteristics of uranium as a fuel. Previous investigators (Refs. 1, 2, and 3) in attempting to evaluate these properties of uranium have found it necessary to assume values for ionization potentials other than the first, for which a value near 6 e.v. (Refs. 4, 5, and 6) seems to be rather well established. In general, the values assumed for the ionization potentials above the first have been based on interpretations of trends in heavy elements reported in the literature rather than on experimental data or detailed calculations for uranium. Because of the effect of the ionization potentials on those physical properties which determine the feasibility of using uranium as a fuel, improved estimates of these potentials were necessary.

Owing to the enormous experimental problems involved and the difficulty of interpreting the extremely complex spectrum of uranium, it was considered more reasonable to estimate the higher ionization potentials by an approximate theoretical method. The details of the approximate quantum mechanical method which was used and the results obtained therewith are described in the following sections.

METHOD

In all time-independent problems of quantum mechanics, the central problem is obtaining a solution to Schrodinger's Equation

$$H\psi_n = E_n\psi_n$$

where H is the Hamiltonian operator for the system and E_n and ψ_n are the corresponding eigenvalues and eigenfunctions of the system in the quantum state denoted by n . Exact solutions of this equation for atomic states exist only for the isoelectronic series of the hydrogen atom; for all other atomic systems, only an approximate solution is possible. The expectation value for the energy in the quantum state, n , of the system is given by

$$E_n = \frac{\int \psi_n^* H \psi_n d\tau}{\int \psi_n^* \psi_n d\tau}$$

If the expectation value of the energy for an atom in its ground state configuration and the expectation value of the energy for the ground state configuration of the first positive ion of that atom are calculated, the ionization potential

(I.P.) of the atom will be the difference between these two expectation values. Letting the subscript o designate the ground state, then the ionization potential of neutral uranium is given by

$$\text{I.P.} = |E_o \text{ (atom)} - E_o \text{ (+ ion)}|$$

A similar expression exists for each of the successively higher ionization potentials. In this study, the expectation value of the ground state energy for the atom and ions was obtained in three steps. In the first step only the average energy of the electrons was obtained, without regard to the splitting of energy levels in the ground state configuration of the atom or ion. In the second step, the core energy obtained from the first step was used as a basis for a more accurate calculation of the energy in which the splitting of the energy levels in the ground state configuration was accounted for. Further refinements to the calculation, which were obtained in step three, were the inclusion of relativistic corrections. Of the corrections added to the average energy, those obtained from step two are by far the more important. This is particularly true for uranium which has an extremely complex spectrum in which the energy levels for a given configuration may be widely spaced and, in fact, may overlap the levels of another configuration. It is this feature which precludes the use of spectral data to obtain the higher ionization potentials. The effects due to changes in the core electrons (relativistic mass change, spin-orbit coupling, and Darwin correction) can be expected to be relatively unimportant since the effective nuclear charge (or scaled nuclear charge as used here) will change by a very small amount for the core electrons in going from the n to the n + 1 ionized state. Consequently, the relativistic corrections which, by the present method, are based upon the scaled nuclear charges obtained from the non-relativistic Hamiltonian will, similarly, be changed by only a very small amount. Hence, the relativistic correction terms which are added to the energy of the atom and ion are very nearly equal. The first ionization potential, which is just the difference between the energies of the atom and ion will, therefore, be changed by only the difference in the two correction terms. This argument could also be made for any higher ionization potential considered in this study.

The mathematical formulation is particularly simple when only the electrostatic energy or the average energy for a configuration is considered. It was this average energy and the corresponding approximate eigenfunctions which were obtained in the first stage of obtaining a solution for the ionization potentials of uranium. Several methods are available for obtaining these approximate eigenfunctions including three which were considered in detail.

The first of these, a simplified Hartree-Fock-Slater approximation (Ref. 7) predicted the removal of a 7s electron from the $6d5f^37s^2$ outer shells to form normal U(II). (Note: The ground state uranium atom is designated as U(I) and the successive ionization levels as U(II), U(III), etc.). However, the normal state of U(II) is generally accepted as having a $5f^37s^2$ configuration which results from the removal of a 6d electron. The simplified Hartree-Fock-Slater

method was therefore ruled out as being too crude an approximation for this study. The second method, a more accurate Hartree-Fock treatment (Ref. 8) which includes spin-orbit and relativistic effects, does indeed predict the correct configuration for U(II). This approach may be quite exact in many cases, but has the disadvantage of requiring a great amount of computation time. This approach was therefore rejected. The third method, a perturbation-variation method due to Layzer (Ref. 9) was chosen because of its relative mathematical simplicity, which indicated that less computation time would be required than with the second method, and also because of the success with which the method had been used by Naqvi and Victor (Ref. 10), to calculate approximate wave functions and energy levels, for both ground and excited states for all the atoms and the first 20 positive ions along the corresponding isoelectronic series which contain from three to fifty-five electrons. Their results were in good agreement with Hartree-Fock calculations where comparison was possible and, in some cases (for the smaller systems), yielded better values for the energy. The theory of this perturbation-variation method is described in Appendix I. A description of the computer program developed to perform the calculation is presented in Appendix II.

After the total average energy for a given electron configuration had been obtained by this perturbation-variation approach, the optimized one-electron orbitals (hydrogen-like orbitals) obtained from this approach were used to construct a properly antisymmetrized wave function for the valence electrons in the field of a central core defined by the average energy calculation. (Electrons in closed shells do not contribute to the splitting in the electronic energy levels and the core electrons could therefore be ignored except for their effect on nuclear charge.) This wave function was then used in a separate proprietary UAC computer program, which had been previously developed by UARL as part of its internal research program, to determine the relative separations of the energy levels for the various possible sublevels of the electronic energy state. The analysis upon which this program is based is described in Ref. 11.

Relativistic corrections were calculated for the atom using the formulas given by Herman and Skillman (Ref. 7). These formulas allow for mass, Darwin, and spin-orbit corrections to the energy. They are based upon the use of hydrogenic orbitals as the basis set for the wave function and treat the relativistic corrections as a first order perturbation. The correction terms by this first order perturbation calculation are correct to order γ^2 where γ is the fine structure constant ($= 1/137.037$). The ionization potentials for all ions of interest were calculated both with and without these relativistic corrections.

PROCEDURE

Ground state configurations for uranium and its first four positive ions, based on an analysis of their spectra, have been proposed in the literature (Ref. 12). Because of the enormous difficulty in analyzing the spectra for a member of the rare earth series, however, the proposed configurations are subject to question. For this reason, verification of the proposed configurations was attempted as part of this study.

In order to verify the proposed electronic configuration for a particular ion, several of the most probable electronic configurations for that ion were assumed and the total average energy (electrostatic energy) for each of these configurations was then calculated by the perturbation-variation approximation. For each specified configuration of the atom or ion of interest, the scaled nuclear charge was calculated by the perturbation-variation method. (The scaled nuclear charge is defined as

$z_\alpha = \frac{2}{n_\alpha} (z - s_\alpha)$ where n_α is the principle quantum number and s_α is the screening constant for the electron shell designated by α , and z is the true nuclear charge.) By an iterative procedure, the values of the scaled nuclear charges were varied until the field which was set up by these charges was consistent with the values of the charges. Since an iterative scheme was used, it was necessary to set up some criteria to determine when the convergence of the scaled nuclear charge had been completed. The criteria which was decided upon was that values of the scaled nuclear charges determined in two successive iterations should differ by no more than .0001. This criteria was maintained for all calculations. After this convergence criteria had been satisfied, the average energy for the atom (or ion) was determined by the simple relation

$$W = -\frac{1}{8} \sum_\alpha q_\alpha z_\alpha^2 \quad (1)$$

where q_α is the number of electrons in the electron shell designated by α , and z_α is the scaled nuclear charge for that shell. The summation is taken over all shells which contain electrons. Ideally, this procedure would yield a sequence of values of average energy for a number of specified configurations for the atom or ion, with the lowest energy corresponding to the ground state configuration. However, the present method of calculation is sufficiently inexact that our results were sometimes in disagreement with the ordering of the levels proposed from interpretation of spectral studies. It was then necessary to use other criteria to determine which of the two was most likely to be correct. The additional criteria which were used were: (1) the agreement of either our calculations or the results of spectral analysis with the Hartree-Fock calculations (Ref. 8); and (2) the regular behavior of the core energy as electron was removed to form the proposed configuration. It was expected that the core energy would increase in a near-linear fashion as the valence electrons were removed. Since the lowest configurations for both U(I) and U(II) are fairly well established, the calculations for these two

systems give an approximate measure of how much the core energy should increase with the removal of each successive electron (Fig. 1). Since the removal of the first valence electron had increased the core energy by about 2.5 Hartree units (1 Hartree = twice the ionization potential of the hydrogen atom), the removal of the second electron was therefore expected to further increase the core energy by approximately 2.5 Hartree units. It should be emphasized that this method for determining the lowest configuration is intimately tied up with the energy calculation itself and was not a method which permitted the determination of the configuration before the energy calculation was completed.

For the ions, U(III) and U(V), the calculated total average energies led to the prediction of a configuration in disagreement with the configuration of Ref. 12. For the U(III) ion, it had been assumed that the electronic configuration would be a radon core for the core atoms plus one of the three possible configurations: (1) $5f^37s$, (2) $5f^27s^2$, or (3) $5f^36d$ for the outer electrons. Of these three configurations, the second one produced the lowest average energy; it was, in fact, about 3.9 electron volts below the average energy for U(II). Upon examination of the wave function for this configuration, however, it was noted that the core electrons were changed drastically from those calculated from configurations (1) or (3). This strongly indicated that the calculation for configuration (2) should not be considered valid. To verify this conclusion, calculations were carried out considering only the valence electrons for the three configurations with the same computer program which was used to determine the splitting of the levels. These calculations indicated that configuration (2) was an excited state of the system. In addition, the near-linear increase of the core energy as the valence electrons were removed was satisfied by both the $5f^37s$ and the $5f^36d$ configurations, but this trend was not satisfied by the $5f^27s^2$ configuration, again indicating that it was not the lowest configuration for this ionization level. The choice of the $5f^37s$ configuration rather than the $5f^36d$ was then confirmed by both the averaged energy calculation and the more exact calculation which considered only valence electrons. This choice is in disagreement with the assigned configuration of Ref. 12, but agrees with the implied configuration of Ref. 13.

The results of the perturbation-variation approach also failed to agree with the spectral prediction of Ref. 12 for the lowest configuration for U(V). The suggestion is made in Ref. 12 that U(V) would be produced in its ground state by the removal of a 5f electron from U(IV), the 6d and 7s electrons having all been removed. The treatment of Ref. 8 also suggests the removal of a 5f electron. Our results, however, indicated that a 6p electron would be released from the core prior to the removal of a 5f electron. To establish whether the 6p or 5f electron lies lower in energy, calculations were performed on two possible configurations using the exact analysis with splitting of energy levels, first on the configuration $6p^25f^2$ and second on the configuration $6p5f^3$. It was not necessary to consider the more complete configurations $6p^55f^3$ and $6p^65f^2$ in this calculation. Since the p shell can hold only 6 electrons, four of which are paired, the configuration $6p^55f^3$

and $6p5f^3$ and the $6p^65f^2$ and $6p^25f^2$ configurations can be constructed to be equivalent insofar as the splitting of the energy levels is concerned. The $6p^25f^2$ configuration was lower in energy, in agreement with the spectral assignment of Ref. 12. Therefore, the perturbation-variation method was abandoned and the lowest configuration was taken to be $5f^2$. To get a value for the core energy for U(V), the scaled nuclear charges obtained from the calculation for a $6p^55f^3$ configuration were used and the summation in Eq. (1) carried out over the desired $6p^65f^2$ core. Some error was introduced in this manner, but the increase in core energy versus the degree of ionization fell very close to the expected near-linear behavior.

Since the perturbation-variation procedure had predicted incorrectly the energy ordering for 6p and 5f electrons, it was no longer possible to obtain a rigorous variational calculation to determine the probable electronic configurations for U(VI). It was necessary, therefore, to assume a configuration for U(VI) which, with the help of Ref. 8, was taken to be $5f$.

The core energy for U(VI) was determined in a more approximate manner. Both the maximum and minimum change in core energy in going from one ion to the next most positive ion was determined from the data on the neutral atom and first four ions. By adding each of these quantities to the core potential obtained for U(V), limits for the maximum and minimum value of the core potential for U(VI) were set. These limits are indicated in Fig. 1. The value for the core potential which was used to determine the average energy for U(VI) was taken as the arithmetic mean of the maximum and minimum values defined by this method. The difference between the two limits is only about 11 e.v., so that the error introduced by this approximation is at most about 6 e.v., if the linear extrapolation is valid. The ground state configurations chosen for the atom and ions are summarized in column I of Table I.

After the above calculations had been completed, the energy levels for the various possible sublevels of the selected ground state configurations were calculated using a properly antisymmetrized wave function for the valence electrons only, based upon a representation using the optimized screened hydrogenic orbitals from the perturbation-variation calculation. An existing proprietary UAC computer program (Ref. 11) was used in carrying out this phase of the calculation. To match the effect of the core electrons which were left out, an effective charge was needed; this effective charge was specified by a single parameter, the magnitude of which was fixed at three different values, which corresponded to a first ionization potential of the atom being calculated as 6.11 e.v. (experimental - Ref. 6), 5.76 e.v. (approximate screened hydrogenic), and 4.39 e.v. (Hartree-Fock-Slater approximation - Ref. 8). No optimization of the one-electron orbitals was performed during this stage of the calculation.

The optimized scaled nuclear charges obtained from the perturbation-variation calculation were used to calculate the relativistic corrections to the total energy using the formulas given by Herman and Skillman (Ref. 7). The results of the present calculations both with and without these corrections are given in Table I.

RESULTS AND DISCUSSION

The converged values of the scaled nuclear charges for neutral uranium and the first three positive ions are listed in Table II. The scaled nuclear charges for U(V) and U(VI) are not included here, since the perturbation-variation method had failed to predict the correct ordering of the energy levels for U(V).

It may be seen from Table II that these scaled nuclear charges do not change by large amounts in progressing from one ionic species to the next species with one higher degree of ionization. The scaled nuclear charges indicate that the 6s and 6p shells contract very rapidly as the degree of ionization increases; the other closed shells are affected to a considerably less degree, the general trend being toward a slight expansion rather than a contraction as observed for the 6s and 6p shells. The behavior of the 5f shell is particularly interesting since, with only three electrons in the shell, it may be considered as one of the valence shells. Yet the removal of the 6d and 7s electrons results in the 5f shell remaining almost unaffected. This indicates that the 5f electrons are buried deep in the core.

In every theoretical determination of the ground state energy some errors are introduced just by the approximation method used to carry out the calculation. The largest error introduced in this way by the present calculation is that due to correlation effects. Since such effects are well understood and are discussed in advanced texts on atomic structure calculations (e.g., Ref. 14) they will not be discussed here. Only those errors which have been introduced within the framework of the various approximations used will be discussed.

The errors introduced into the calculation of the first three ionization potentials are probably not serious. Some improvement could have been obtained by treating the level splitting within the perturbation-variation method. This would have allowed complete optimization of the scaled nuclear charges. Even so, it is not felt that any serious error was introduced by the approach which was used.

The relativistic corrections were only minor corrections, as expected, for the first three ionization levels; however, the ionization potential of U(IV) was decreased by some 7 e.v. when these corrections were made. Since these corrections are made using the scaled nuclear charges obtained from the nonrelativistic calculation, and since the scaled nuclear charges which were used were those obtained for the $6p^5 5f^3$ configuration and not the ones obtained for the $6p^6 5f^2$ configuration, some error is introduced. It is felt that the relativistic corrections for this case have been overestimated; consequently, the suggested value (Table I) for this ionization potential was chosen more in accord with the nonrelativistic values.

Values of the uranium ionization potentials derived in this study for U(II) and U(III) were used to recalculate the species concentrations, coefficients of

viscosity and diffusion, and related quantities which were previously reported (Refs. 1 and 2) for a number of equilibrium mixtures of hydrogen and uranium. Revised values for these quantities are shown in Tables III-XIII at pressures of 100, 500, and 1000 atm, temperatures of 20,000, 60,000, and 100,000 K, and for P_{FUEL}/P ratios of 0.09, 0.1, 0.233, 0.367, 0.5, 0.633, 0.767, and 0.9. At the time these calculations were initiated, the relativistic corrections to the energies had not been computed so a set of preliminary values were used. These values are indicated in the fourth column of Table I. These values are sufficiently close to the values finally suggested that the error introduced by the discrepancy is expected to be quite small (Ref. 15). The effect of the revised ionization potentials upon the relative concentrations of the various uranium species is typified by the behavior of the curves shown in Fig. 2 where these concentrations are plotted against temperature for a pressure of 1000 atm and a P_{FUEL}/P ratio of 0.5 using both the new data and the old data from Ref. 1. The data in Table III and Fig. 2 indicate that, as would be expected, the increased values for the ionization potentials of U(II) and U(III) causes the uranium ions of the lower valences to play an increased role in the determination of the properties of a given mixture out to higher temperatures than had been indicated previously. The changes in concentrations are, however, most significant in the regions of lower temperature; at the highest temperatures considered the uranium mixtures are again predominantly U^{+++} and electrons. A complete evaluation of the effects of the revised values of the ionization potential on the concentrations of more highly ionized states has not been possible since the computer program used for making these calculations (Ref. 3) is able to consider only states through U^{+++} . The trends shown in Fig. 2 indicate that states above U^{+++} will be much less important than had previously been considered possible even at temperatures near 10^5 K. Nevertheless some contribution from states above U^{+++} may still occur near this temperature.

The changes in the concentrations are reflected in the recomputed values of the transport data. Thus, without exception, all of the quantities reported in Tables IV-XIII are seen to agree well with the corresponding values in Refs. 1 or 2 at 100,000 K, but to differ more significantly from these corresponding values at 20,000 K. (Reference 2 was published subsequent to the release of Ref. 1 and contains values of the mixture properties such as viscosity, effective binary diffusivity, and Schmidt number which were revised when more sophisticated calculation procedures became available. The data contained therein are, however, still based on the old values for the uranium ionization potentials.) For those properties such as component viscosities (Table IV) and binary interionic diffusivities (Table V) which are not strongly dependent upon composition, the changes are, for the most part, small. However, for those properties such as mixture viscosity (Table VI) and effective hydrogen-uranium binary diffusivity (Table VIII), which are strongly composition dependent, the changes are more significant, some of the values increasing by as much as a factor of 3 1/2 at the lowest pressure, temperature, and P_{FUEL}/P ratios studied. Changes in the Schmidt number which is, in general, also strongly composition dependent, are, however, much less marked due to the tendency for viscosity and diffusivity to both increase in the same direction. This is

indicated by the curves in Fig. 3 which show that the broad range of Schmidt numbers encountered does not change significantly, although the values for a specified temperature, pressure and fuel partial pressure may change by as much as 50% in some cases. Schmidt numbers and effective binary diffusivities are not reported for the fuel-rich mixtures at 20,000 °K. As can be seen from Fig. 2, at this temperature the changes brought about in the concentrations of the uranium ions of higher valency by the use of new values for the corresponding ionization potentials are rather severe. This causes spurious values for the effective gradients calculated for these species in the fuel-rich mixtures at this temperature, thereby leading to anomalous values for D_{eff}^{U-H} and the Schmidt number. The use of more closely spaced points in the calculation of the concentration gradients should eliminate this problem.

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LIST OF SYMBOLS

a_0	One Bohr radius ($\approx .52 \times 10^{-8}$ cm)
b_i	The i th member of a set of expansion coefficients
$C_{L_\alpha L_\beta}^k$	Integral over three Legendre functions
D_{ij}	Binary diffusivity describing mutual diffusion of species i and j , ft^2/sec
$D_{\text{eff}}^{\text{U-H}}$	Effective binary diffusivity describing mutual diffusion of hydrogen-based and uranium-based constituents, ft^2/sec
D_L	Binary diffusivity calculated using a Coulomb potential with a cutoff at the Debye length, ft^2/sec
D_{SC}	Binary diffusivity calculated using a shielded Coulomb potential, ft^2/sec
D_R	Binary diffusivity calculated using a Coulomb potential with a cutoff at the outer radius of an ionic cell, ft^2/sec
D_{ij}	Coefficient of diffusion in a multicomponent mixture, ft^2/sec
$D_{i-\text{MIX}}^m$	Effective mass diffusivity for species i , $\frac{\text{lb}}{\text{lb mole}} \cdot \frac{\text{ft}^2}{\text{sec}}$
E_n	Eigenvalue of the Hamiltonian operator, specifying the expectation value of the energy for the quantum state labeled by n , atomic units
$E(N,Z)$	One-electron energy operator showing explicit dependence upon number of electrons, N , and atomic number, Z , atomic units
$F^\circ(\alpha\beta)$	Slater coulomb integral between electrons in shells α and β
$G^k(\alpha\beta)$	Slater exchange integral between electrons in shells α and β
H	Quantum mechanical Hamiltonian operator
$H(N,Z)$	Hamiltonian operator showing explicit dependence upon number of electrons, N , and atomic number, Z .
i, j, k	Used as summation indices

LIST OF SYMBOLS
(cont'd)

I.P.	Ionization potential, electron volts
ℓ	Angular momentum quantum number
ℓ_a	Angular momentum quantum number for electron in shell denoted by a
m_i	Particle mass of species i , lb/particle
m_i^{eff}	Effective particle mass of pseudo-species i , lb/particle
M_i	Molecular weight of species i , lb/lb-mole
n	Total number density of particles in a system, $\frac{\text{particles}}{\text{cm}^3}$
n_a	Principle quantum number of shell a
n_i	Number density of species i , particles/cm 3
n_{ions}	Number density of ions, particles/cm 3
N	Number of electrons on atom or ion
N_{sc}	Schmidt number
o	Subscript indicating set of quantum numbers for the ground state atom or ion
P	Parity
P	Total pressure, atm
P_{FUEL}	Pressure of fuel-based constituents, atm
q_a	Number of electrons in shell a
r_i	Radial coordinate of electron labeled by i , Bohr radii
r_{ij}	Interparticle separation of electrons labeled by i and j , Bohr radii
R	Contribution to the two-electron energy that depends on quantum numbers other than the principle and angular momentum quantum numbers

LIST OF SYMBOLS
(cont'd)

S	Total spin for two electrons
S_α	Screening constant for electrons in shell specified by the α set of quantum numbers
T	Temperature, K
U(I)	Neutral uranium atom
U(II), U^+	Singly ionized uranium
U(III), U^{++}	Doubly ionized uranium
$U(\alpha, \beta)$	Matrix defined by Eq. (11b) of Appendix II
$V(N)$	Two-electron potential energy operator for an N electron atom, Hartree
$V_{(n), pSL}$	Eigenvalues of the two-electron interaction matrix
W	Calculated average energy, Hartree
W(S)	Calculated average energy showing explicit dependence on the set of screening constants, Hartree
Z_α	Scaled nuclear charge ($= \frac{2}{n_\alpha} (Z - S_\alpha)$)
Z	Atomic number or nuclear charge
Z_α	Effective nuclear charge for electrons in the shell denoted by α
α OR β	Set of numbers specifying the principle and angular momentum quantum numbers for an electron
$\delta_{\alpha\beta}$	Kronecker delta ($= 1$ if $\alpha = \beta$, $= 0$ if $\alpha \neq \beta$)
γ	Fine structure constant ($= 1/137.037$)
Δ	Increment
η_i	Viscosity of component i, lb/ft-sec

LIST OF SYMBOLS
(cont'd)

η_{ij}	Binary viscosity term used in calculation of mixture viscosity for a binary system, lb/ft-sec
η_L	Viscosity calculated using a coulomb potential with a cutoff at the Debye length, lb/ft-sec
η_{SC}	Viscosity calculated using a shielded-coulomb potential, lb/ft-sec
η_R	Viscosity calculated using a coulomb potential with a cutoff at the outer radius of an ionic cell, lb/ft-sec
η_{MIX}	Mixture viscosity, lb/ft-sec
ρ	Total mass density, lb/ft ³
Σ	Summation symbol
ψ_n	Wave function for system in quantum state specified by the set of quantum numbers n
ψ_n^*	Complex conjugate of ψ_n
∇_i^2	Laplacian operator
$\frac{\partial}{\partial x}$	Partial derivative with respect to the independent variable x (x is arbitrary)

APPENDIX I

LAYZER'S METHOD

The method for determining the electronic energy of an atom which was introduced by Layzer (Ref. 9) and used in the present study is described in the following paragraphs. In this method, a model is assumed such that each electron of the system is considered to move in its own stationary orbit in a central field produced by some effective nuclear charge and the interelectron repulsion is treated as a perturbation. The wave equation for the system of N particles then separates into N , uncoupled, hydrogen-like equations and the total energy is just the sum of the expectation values of the N one-electron Hamiltonians. A minimum value for the total energy is determined variationally.

As in all time-independent problems in quantum mechanics, Layzer's approach is concerned with the solution of Schrödinger's equation.

$$H\psi_n = E_n \psi_n \quad (1)$$

where H is the Hamiltonian operator for the system and E_n and ψ_n are the corresponding eigenvalues and wavefunctions of the system, for the quantum state denoted by n . Exact solutions of Eq. (1) exist for the isoelectronic series of the hydrogen atom only; for all other systems, only an approximate solution is possible. Following Layzer, the development presented here is restricted to the use of a non-relativistic Hamiltonian for an atom or ion containing a nuclear charge Z and N electrons. With these restrictions, the Hamiltonian is of the form (in atomic units)

$$\begin{aligned} H(N, Z) &= \sum_i^N \left(\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right) + \sum_{i < j=1}^N \frac{1}{r_{ij}} \\ &= E(N, Z) + V(N) \end{aligned} \quad (2)$$

where

$$E(N, Z) \equiv \sum_i^N \left(\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right)$$

$$V(N) \equiv \sum_{i < j}^N \frac{1}{r_{ij}}$$

If the unit of length is changed from a_0 (the Bohr radius) to a_0/z the Hamiltonian may be expressed as

$$H(N, z) = z^2 \left\{ E(N, 1) + z^{-1} V(N) \right\} \quad (3)$$

Using $\lambda = z^{-1}$ as the expansion parameter by which the system wavefunction and eigenvalues are expanded in the conventional perturbation scheme yields a hydrogenic eigenvalue and eigenvector as the leading term in both expansions as indicated in Eqs (4).

$$\Psi = |H'\rangle = \sum_{n=0}^{\infty} z^{-n} |n\rangle \quad (4a)$$

$$E = H' = z^2 \sum_{n=0}^{\infty} b_n z^{-n} \quad (4b)$$

Since this is true, it is obvious that b_0 must then be of the form

$$b_0 = - \sum_{i=1}^N \frac{1}{2n_i^2}$$

to yield the sum of hydrogenic Hamiltonians, while the terms b_1, b_2, \dots are identified with the matrix $V(n)$ whose elements have been evaluated in a representation based upon hydrogenic orbitals. This is the conventional perturbation theory, which Layzer altered slightly in order to allow for the screening experienced by the electrons. If the effective nuclear charge, z_α , and the screening parameters, S_α , for the electron shell designated by α are defined by the relationship

$$z_\alpha = z - S_\alpha \quad (5)$$

then the expectation value for the hydrogen-like Hamiltonian is $\langle \alpha | E(z) | \alpha \rangle$. If there are q_α electrons in the shell designated by α , then the total one-electron energy for that shell is $q_\alpha \langle \alpha | E(z) | \alpha \rangle$, while the sum of

such energies over all occupied shells is just

$$\begin{aligned}
 \sum_{\alpha} q_{\alpha} \langle \alpha | E(z) | \alpha \rangle &= \sum_{\alpha} q_{\alpha} \left\langle \alpha \left| \frac{1}{2} p_{\alpha}^2 - \frac{z}{r} \right| \alpha \right\rangle \\
 &= \sum_{\alpha} q_{\alpha} \left\langle \alpha \left| \frac{1}{2} p_{\alpha}^2 - \frac{z_{\alpha}}{r} - \frac{s_{\alpha}}{r} \right| \alpha \right\rangle \\
 &= \sum_{\alpha} q_{\alpha} \left\{ \langle \alpha | E(z_{\alpha}) | \alpha \rangle - s_{\alpha} \langle \alpha | \frac{1}{r} | \alpha \rangle \right\} \\
 &= \sum_{\alpha} q_{\alpha} \left\{ - \frac{z_{\alpha}^2}{2n_{\alpha}^2} - s_{\alpha} \frac{z_{\alpha}}{n_{\alpha}^2} \right\} \\
 &= - \sum_{\alpha} \frac{q_{\alpha} (z^2 - s_{\alpha}^2)}{2n_{\alpha}^2}
 \end{aligned} \tag{6}$$

Considering the Coulombic repulsion between the electrons as a perturbation and denoting as $V_1 (\dots z_{\alpha} \dots)$ the lowest eigenvalue of the interaction matrix, the total energy for the system may be written simply as

$$W(s) = - \sum_{\alpha} \frac{q_{\alpha} (z^2 - s_{\alpha}^2)}{2n_{\alpha}^2} + V_1 (\dots z_{\alpha} \dots) \tag{7}$$

where the matrix elements $V_1 (\dots z_{\alpha} \dots)$ are evaluated using screened hydrogenic orbitals (hydrogenic orbitals with nonintegral values of Z). In order to find the set of screening parameters which minimizes $W(s)$, it is necessary to set

$$\frac{dW(s)}{ds_{\alpha}} = 0 = \frac{q_{\alpha} s_{\alpha}}{n_{\alpha}^2} + \frac{\partial V_1}{\partial s_{\alpha}} = \frac{q_{\alpha} s_{\alpha}}{n_{\alpha}^2} - \frac{\partial V_1}{\partial z_{\alpha}}, \text{ (for all } \alpha \text{)} \tag{8}$$

But, using Euler's relations for homogeneous functions, V_1 may be expressed as

$$V_1 = \sum_{\alpha} z_{\alpha} \frac{\partial V_1}{\partial z_{\alpha}} = \sum_{\alpha} \frac{q_{\alpha} s_{\alpha} z_{\alpha}}{n_{\alpha}^2}$$

These eigenvalues are eigenvalues of the matrices $V_{(n),PSL}$, where pSL is the set of quantum numbers specifying the parity, spin, and angular momentum, respectively, and n indicates that the elements connect terms belonging to the same set of radial quantum numbers. The eigenvalue, V_1 , may be written as

$$V_1 = \sum_{\alpha \geq \beta} q_{\alpha \beta} [\alpha \beta] + R \tag{9}$$

where α and/or β designate the quantum state specified by the pair of quantum numbers n and ℓ ; $q_{\alpha\beta}$ is the number of distinct pairs of electrons with one electron drawn from each of the groups α, β ; $[\alpha\beta]$ is the two-electron interaction energy; and R represents contributions that depend on quantum numbers other than n and ℓ .

From Ref. 9

$$q_{\alpha\beta} = \begin{cases} \frac{q_\alpha}{2}, & \alpha = \beta \\ q_\alpha q_\beta, & \alpha \neq \beta \end{cases} \quad (10a)$$

and $[\alpha\beta] = F^\circ(\alpha\beta) - \frac{1}{4} \left(1 + \frac{\delta_{\alpha\beta}}{4\ell_\alpha + 1} \right) \sum_k c_{\ell_\alpha \ell_\beta k} G^k(\alpha\beta) \quad (10b)$

where $F^\circ(\alpha\beta)$ and $G^k(\alpha\beta)$ are the so-called Slater integrals which are evaluated using screened hydrogenic orbitals. With these expressions, then, equation (8) may be written in the form

$$S_\alpha = \frac{n_\alpha^2}{q_\alpha} \frac{\partial V_1}{\partial Z_\alpha} = \sum_\beta (q_\beta - \delta_{\alpha\beta}) U(\alpha\beta) \quad (11a)$$

where $U(\alpha\beta) = \left(1 - \frac{\delta_{\alpha\beta}}{2} \right) n_\alpha^2 \frac{\partial [\alpha\beta]}{\partial Z_\alpha} \quad (11b)$

and

$$\delta_{\alpha\beta} = \begin{bmatrix} 1 & \text{if } \alpha = \beta \\ 0 & \text{if } \alpha \neq \beta \end{bmatrix}$$

Since $U(\alpha\beta)$ is evaluated using the screening parameters S_β (for all values of β including $\beta = \alpha$), a self-consistent set of screening parameters must be obtained to satisfy equation 11. These N coupled linear equations may be solved by an iterative scheme which is far simpler than the set of N coupled integro-differential equations which is encountered in the Hartree-Fock method.

Using this set of screening parameters which satisfied Eq. 11 and substituting the above expression for V_1 into the expression for the minimum energy yields

$$\begin{aligned}
 W(S)_{\text{MIN}} &= - \sum_{\alpha} \frac{q_{\alpha} (z^2 - s_{\alpha}^2)}{2 n_{\alpha}^2} + \sum_{\alpha} \frac{q_{\alpha} s_{\alpha} z_{\alpha}}{n_{\alpha}^2} \\
 &= - \sum_{\alpha} \frac{q_{\alpha} (z - s_{\alpha})^2}{2 n_{\alpha}^2} \\
 &= - \sum_{\alpha} \frac{q_{\alpha} z_{\alpha}^2}{2 n_{\alpha}^2} \\
 &= - \sum_{\alpha} \frac{q_{\alpha} z_{\alpha}^2}{8}
 \end{aligned} \tag{12}$$

APPENDIX II

COMPUTER PROGRAM

A computer program to calculate electronic energies following Layzer's method (Ref. 9) as modified by Naqvi and Victor (Ref. 10) was prepared at UARL.

This program was written in FORTRAN using double-precision arithmetic for an IBM-7094. A listing of the program source deck is presented in Table XIV. The results from this program were checked, using the results of Naqvi and Victor (Ref. 10) which had been obtained with a program coded in single precision for the CDC-1604 computer. These results were in agreement to the eight digits that appeared in the UARL printout for the orbitals with a small number of radial nodes, but did not agree for the orbitals with a large number of nodes. Since the quantity being compared (Table 3.2, Ref. 10) was determined by numerous additions and subtractions of nearly equal numbers, it was understandable that the single precision arithmetic would introduce a round-off error.

The program is written to solve for the set of screening parameters given by equation (11) in Appendix I by an iterative method until a consistent set of parameters results.

The steps used in the iterative scheme are

- (i) Let $z \rightarrow \infty$
then

$$\left(\frac{z_\alpha}{z_\beta} \right) = \frac{\frac{2}{n_\alpha} z_\alpha}{\frac{2}{n_\beta} z_\beta} = \frac{\frac{2}{n_\alpha} (z - s_\alpha)}{\frac{2}{n_\beta} (z - s_\beta)} \longrightarrow \frac{\frac{1}{n_\alpha}}{\frac{1}{n_\beta}}$$

so that

$$z_\alpha^0 = \frac{1}{n_\alpha} \text{ (for all } \alpha \text{)}$$

may be used as an initial value to start the iterative calculation.

- (ii) Evaluate the right side of

$$z_\alpha = \frac{2z}{n_\alpha} - \frac{2}{n_\alpha} \sum_\beta (q_\beta - \delta_{\alpha\beta}) U(\alpha\beta)$$

where $U(\alpha\beta)$ and $\delta_{\alpha\beta}$ are as defined by equation (11) in Appendix I

(iii) Iterate, using the set of values for z_a^i which was obtained from the i^{th} iteration to evaluate the right hand side of the above relation and thus produce the set of values for z_a^{i+1} , until

- (a) i reaches a maximum value, M , read in as input data, or
- (b) convergence was completed by

$|z_a^i - z_a^{i-1}| \leq \epsilon$

where ϵ may be any arbitrarily selected value. Throughout the present calculation a value of $\epsilon = .0001$ was used.

The converged set of scaled nuclear charges obtained for $U(I)$ was used as the initial guess for the scaled nuclear charges for $U(II)$. The iterative process was then carried out as was outlined above for $U(I)$. For each successive ion, the set of scaled nuclear charges of the previous ion (with one less degree of ionization) was used as the initial values to start the iterative process.

The convergence rate of the screening parameters was extremely slow for some of the ionic species. To assist this slow process, plots of the screening parameters versus number of iterations were made and extrapolations for from five to ten iterations ahead of the calculation were performed. These extrapolated values were then read in and from three to six more machine iterations were performed. This process was repeated until the convergence criteria was satisfied.

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TABLE I

CALCULATED IONIZATION POTENTIALS FOR URANIUM

<u>Atomic Configuration</u>	<u>Ionization Potential, e.v.</u>		<u>Suggested Values</u>	
	<u>Non-Relativistic Calculation</u>	<u>Relativistic Calculation</u>	<u>Preliminary*</u>	<u>Final</u>
U(I) $^5L(5f^37s^26d)$ (a)	6.11	6.11	6.1	6.11
	(b)	5.76	5.80	
	(c)	4.39	4.43	
U(II) $^4I(5f^37s^2)$ (a)	17.1	17.9	17.1	17.5
	(b)	16.6	17.5	
	(c)	15.2	15.9	
U(III) $^5I(5f^37s)$ (a)	38.8	36.2	38.8	37.5
	(b)	38.3	35.8	
	(c)	36.8	34.3	
U(IV) $^4I(5f^3)$ (a)	65.6	58.6	65.6	61
	(b)	64.1	57.4	
	(c)	59.6	52.6	
U(V) $^3H(5f^2)$	119	118	---	118

- (a) Screening adjusted to reproduce the experimental value for the first ionization potential (Ref. 6).
- (b) Screened hydrogenic approximation (this calculation).
- (c) Screening adjusted to reproduce the first Hartree-Fock ionization potential (Ref. 8).

* Used to calculate composition and transport properties.

TABLE II

SCALED NUCLEAR CHARGES FOR THE GROUND STATE CONFIGURATIONS OF
NEUTRAL URANIUM AND ITS FIRST THREE POSITIVE IONS

<u>Shell Designation</u>	<u>Species (Configuration)</u>			
	<u>U (I) (5f³6d⁷s²)</u>	<u>U (II) (5f³7s²)</u>	<u>U (III) (5f³7s)</u>	<u>U (IV) (5f³)</u>
1s	182.9136	182.9136	182.9139	182.9142
2s	86.8670	86.8658	86.8644	86.8638
2p	86.9718	86.9712	86.9712	86.9714
3s	51.0886	51.0842	51.0741	51.0678
3p	50.8834	50.8789	50.8734	50.8713
3d	50.7429	50.7425	50.7431	50.7439
4s	30.4516	30.4385	30.4047	30.3859
4p	29.7749	29.7610	29.7362	29.7261
4d	28.5622	28.5625	28.5616	28.5632
4f	27.1099	27.1142	27.1196	27.1238
5s	18.3161	18.2488	18.1187	18.0631
5p	17.5000	17.4390	17.3598	17.3378
5d	15.6338	15.6206	15.5989	15.5977
5f	11.4396	11.4443	11.4271	11.4351
6s	9.0911	9.3812	9.9250	10.2161
6p	8.8599	9.2190	9.6774	9.8789
6d	4.8477			
7s	6.1269	6.1984	6.2328	

CALCULATED COMPOSITIONS FOR EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM

CONCENTRATION (PARTICLES/cm³)

P = 100 ATM

P _{FUEL} /P	n _e	n _{H+}	T = 20,000 DEG K			n _H
			n _{U⁺}	n _{U⁺⁺}	n _{U⁺⁺⁺}	
0.09	1.2778 E19	1.0933 E19	1.0670 E18	3.8926 E17	4.8514 E11	4.9548 E15
0.1	1.2804 E19	1.0767 E19	1.2259 E18	4.0530 E17	4.5774 E11	6.2825 E15
0.233	1.3901 E19	9.3816 E18	3.4823 E18	5.1874 E17	2.6398 E11	9.3873 E16
0.367	1.4927 E19	7.9543 E18	5.8441 E18	5.6431 E17	1.8614 E11	1.0254 E17
0.5	1.5878 E19	6.4954 E18	8.2051 E18	5.8879 E17	1.4433 E11	7.3234 E18
0.633	1.6751 E19	4.9767 E18	1.0566 E19	6.0419 E17	1.1803 E11	5.3600 E18
0.767	1.7520 E19	3.3534 E18	1.2937 E19	6.1485 E17	9.9823 E10	3.5166 E18
0.9	1.8107 E19	1.5802 E18	1.5282 E19	6.2256 E17	8.6642 E10	4.6120 E17
						1.8446 E18
						5.0972 E17
T = 60,000 DEG K						
0.09	6.3834 E18	5.5582 E18	1.8087 E12	5.7078 E15	2.7127 E17	6.8330 E7
0.1	6.4140 E18	5.4972 E18	2.4759 E12	7.0332 E15	3.0089 E17	1.0391 E8
0.233	6.8164 E18	4.6856 E18	3.0470 E13	3.7239 E16	6.8543 E17	2.9722 E9
0.367	7.2159 E18	3.8676 E18	1.1591 E14	9.0151 E16	1.0560 E18	1.3080 E16
0.5	7.6070 E18	3.0554 E18	2.8562 E14	1.6342 E17	1.4081 E18	9.6305 E15
0.633	7.9931 E18	2.2432 E18	5.6512 E14	2.5594 E17	1.7458 E18	5.9512 E10
0.767	8.3770 E18	1.4244 E18	9.8079 E14	3.6736 E17	2.0723 E18	6.5522 E15
0.9	8.7536 E18	6.1152 E17	1.5471 E15	4.9484 E17	2.3836 E18	3.9373 E15
						3.1216 E11
						1.8761 E15
						4.6626 E14
T = 100,000 DEG K						
0.09	3.8348 E18	3.3389 E18	1.1400 E9	4.8331 E13	1.6530 E17	7.5051 E3
0.1	3.8533 E18	3.3022 E18	1.5637 E9	5.9666 E13	1.8366 E17	1.1439 E4
0.233	4.0983 E18	2.8143 E18	1.9772 E10	3.2380 E14	4.2778 E17	3.3698 E5
0.367	4.3451 E18	2.3227 E18	7.7234 E10	8.0306 E14	6.7358 E17	2.0733 E6
0.5	4.5899 E18	1.8347 E18	1.9523 E11	1.4900 E15	9.1739 E17	7.1399 E6
0.633	4.8347 E18	1.3468 E18	3.9598 E11	2.3873 E15	1.1610 E18	1.8333 E7
0.767	5.0812 E18	8.5508 E17	7.0417 E11	3.5038 E15	1.4064 E18	5.9903 E14
0.9	5.3257 E18	3.6701 E17	1.1372 E12	4.8225 E15	1.6497 E18	3.9502 E7
						7.4854 E7
						1.7478 E16
						1.7142 E16
						1.3080 E16
						9.6305 E15
						1.3962 E15
						1.8924 E15
						2.4346 E15
						2.4862 E16

TABLE III (CONT'D)
 CALCULATED COMPOSITIONS FOR EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM
 CONCENTRATION (PARTICLES / CM³)

		P = 500 ATM						T = 20,000 DEG K						T = 60,000 DEG K						T = 100,000 DEG K																																											
	P _{FUEL} /P	n _e	n _{H+}	n _{U+}	n _{U⁺⁺}	n _{U⁺⁺⁺}	n _H	n _U	n _{U⁺⁺}	n _{U⁺⁺⁺}	n _H	n _U	n _{U⁺⁺}	n _{U⁺⁺⁺}	n _H	n _U	n _{U⁺⁺}	n _{U⁺⁺⁺}	n _H	n _U	n _{U⁺⁺}	n _{U⁺⁺⁺}	n _H																																								
0.09	4.8634 E19	4.6788 E19	1.0670 E18	3.8926 E17	4.8514 E11	4.9548 E15	7.3388 E19	0.1	5.5665 E19	4.6282 E19	8.2051 E18	5.8879 E17	1.4433 E11	1.9372 E17	7.2569 E19	0.233	6.0795 E19	3.9608 E19	1.9921 E19	6.3305 E17	6.8724 E10	1.0621 E18	6.1518 E19	0.367	6.5739 E19	3.3002 E19	3.1444 E19	6.4669 E17	4.5434 E10	2.5904 E18	5.0101 E19	0.5	7.0424 E19	2.6525 E19	4.2293 E19	6.5325 E17	3.4226 E10	4.7052 E18	3.8698 E19	0.633	7.4852 E19	2.0067 E19	5.3470 E19	6.5714 E17	2.7589 E10	7.3714 E18	2.7212 E19	0.767	7.8953 E19	1.3461 E19	6.1172 E19	6.5973 E17	2.3169 E10	1.0576 E19	1.5835 E19	0.9	8.2374 E19	6.4954 E18	7.4556 E19	6.6155 E17	2.0053 E10	1.4236 E19	5.3600 E18
0.09	3.1812 E19	2.7711 E19	2.1024 E14	1.3354 E17	1.2775 E18	3.9458 E10	2.4712 E17	0.1	3.1960 E19	2.7408 E19	2.8562 E14	1.6342 E17	1.4081 E18	5.9512 E10	2.4288 E17	0.233	3.3866 E19	2.3366 E19	3.2052 E15	7.9490 E17	2.9691 E18	1.5407 E12	1.8850 E17	0.367	3.5695 E19	1.9293 E19	1.1254 E16	1.7668 E18	4.2725 E18	8.4504 E12	1.3819 E17	0.5	3.7437 E19	1.5246 E19	2.5866 E16	3.0354 E18	5.3648 E18	2.6276 E13	9.4924 E16	0.633	3.9122 E19	1.1197 E19	4.8110 E16	4.4866 E18	6.3013 E18	6.1502 E13	5.7561 E16	0.767	4.0771 E19	7.1134 E18	7.8968 E16	6.1099 E18	7.1197 E18	1.2167 E14	2.6804 E16	0.9	4.2366 E19	3.0554 E18	1.1849 E17	7.8494 E18	7.8313 E18	2.1324 E14	6.5522 E15
0.09	1.9165 E19	1.6685 E19	1.4234 E11	1.2071 E15	8.2575 E17	4.6852 E6	3.2973 E16	0.1	1.9253 E19	1.6501 E19	1.9523 E11	1.4900 E15	9.1739 E17	7.1399 E6	3.2441 E16	0.233	2.0482 E19	1.4064 E19	2.4646 E12	8.0747 E15	2.1341 E18	2.0998 E8	2.5376 E16	0.367	2.1715 E19	1.1607 E19	9.6122 E12	1.9997 E16	3.3559 E18	1.2897 E9	1.8741 E16	0.5	2.2938 E19	9.1696 E18	2.1259 E13	3.7051 E16	4.5647 E18	4.4336 E9	1.2769 E16	0.633	2.4159 E19	6.7316 E18	4.9128 E13	5.9277 E16	5.7697 E18	1.1365 E10	7.5766 E15	0.767	2.5386 E19	4.2743 E18	8.7226 E13	8.6874 E16	6.9798 E18	2.4445 E10	3.6466 E15	0.9	2.6605 E19	1.8347 E18	1.4065 E14	1.1940 E17	8.1770 E18	4.6244 E10	9.8501 E14

TABLE III (CONT'D)
 CALCULATED COMPOSITIONS FOR EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM
 CONCENTRATION (PARTICLES / CM³)

P = 1000 ATM

P _{FUEL} / P	n _e	n _{H⁺}	n _{U⁺}	n _{U⁺⁺}	n _{U⁺⁺⁺}	n _U	n _H
T = 20,000 DEG K							
T = 60,000 DEG K							
0.09	1.1672 E20	1.0019 E20	1.5282 E19	6.2256 E17	8.6642 E10	6.3553 E17	1.3449 E20
0.1	1.1716 E20	9.8870 E19	1.7037 E19	6.2712 E17	7.8855 E10	7.8421 E17	1.3378 E20
0.233	1.2323 E20	8.2160 E19	3.9769 E19	6.5192 E17	3.6506 E10	4.1104 E18	1.1808 E20
0.367	1.2933 E20	6.6448 E19	6.1560 E19	6.5917 E17	2.4112 E10	9.7403 E18	1.0004 E20
0.5	1.3194 E20	5.1391 E19	8.2215 E19	6.6261 E17	1.8243 E10	1.7283 E19	8.0692 E19
0.633	1.4132 E20	3.7972 E19	1.0202 E20	6.6463 E17	1.4791 E10	2.6532 E19	5.8739 E19
0.767	1.4741 E20	2.4875 E19	1.2121 E20	6.6597 E17	1.2500 E10	3.7378 E19	3.5760 E19
0.9	1.5270 E20	1.1783 E19	1.3958 E20	6.6692 E17	1.0885 E10	4.9497 E19	1.3117 E19
T = 100,000 DEG K							
0.09	6.3448 E19	5.5306 E19	1.5471 E15	4.9484 E17	2.3836 E18	5.7667 E11	7.2642 E17
0.1	6.3735 E19	5.4701 E19	2.0853 E15	6.0113 E17	2.6098 E18	8.6237 E11	7.1320 E17
0.233	6.7365 E19	4.6648 E19	2.1439 E16	2.6949 E18	5.1019 E18	2.0332 E13	5.4589 E17
0.367	7.0772 E19	3.8522 E19	7.0551 E16	5.6970 E18	6.9284 E18	1.0416 E14	4.0346 E17
0.5	7.3985 E19	3.0444 E19	1.5427 E17	9.2268 E18	8.3112 E18	3.0750 E14	2.8624 E17
0.633	7.7086 E19	2.2363 E19	2.7569 E17	1.3120 E19	9.4028 E18	6.9065 E14	1.7567 E17
0.767	8.0117 E19	1.4211 E19	4.3771 E17	1.7295 E19	1.0292 E19	1.3206 E15	8.4841 E16
0.9	8.3011 E19	6.1072 E18	6.3875 E17	2.1620 E19	1.1021 E19	2.2498 E15	2.0595 E16
T = 100,000 DEG K							
0.09	3.8312 E19	3.3353 E19	1.1372 E12	4.8625 E15	1.6497 E18	7.4854 E7	9.6828 E16
0.1	3.8491 E19	3.2987 E19	1.9523 E12	1.4900 E15	1.8348 E18	7.1399 E8	9.5198 E16
0.233	4.0948 E19	2.8115 E19	1.9649 E13	3.2198 E16	4.2561 E18	3.3470 E9	7.4269 E16
0.367	4.3413 E19	2.3207 E19	7.6482 E13	7.9595 E16	6.6821 E18	2.0513 E10	5.4705 E16
0.5	4.5851 E19	1.8333 E19	1.9265 E14	1.4721 E17	9.0746 E18	7.0371 E10	3.7947 E16
0.633	4.8285 E19	1.3459 E19	3.8939 E14	2.3511 E17	1.1452 E19	1.8000 E11	2.3693 E16
0.767	5.0729 E19	8.5464 E18	6.9001 E14	3.4396 E17	1.3832 E19	3.8636 E11	1.1356 E16
0.9	5.3150 E19	3.6690 E18	1.1105 E15	4.7193 E17	1.6179 E19	7.2938 E11	2.8794 E15

TABLE IV
 VISCOSITIES OF H⁺, U⁺, U⁺⁺, AND U⁺⁺⁺ IONS
 CALCULATED BY THREE DIFFERENT PROCEDURES
 VISCOSITY IN LB/(FT-SEC)

M	Z	T - DEG K	P = 100 ATM			P = 500 ATM			P = 1000 ATM		
			η_L	η_{SC}	η_R	η_L	η_{SC}	η_R	η_L	η_{SC}	η_R
									$P_{FUEL}/P = 0.09$		
1.0	1.	0.1000E 06	0.11745E-03	0.1731E-03	0.1902E-03	0.2107E-03	0.2086E-03	0.2173E-03	0.2314E-03	0.2289E-03	0.2316E-03
1.0	1.	0.6000E 05	0.6223E-04	0.6158E-04	0.6300E-04	0.7966E-04	0.7832E-04	0.78CE-04	0.9049E-04	0.8919E-04	0.7954E-04
1.0	1.	0.2000E 05	0.8495E-05	0.8364E-05	0.5923E-05	0.1333E-04	0.1339E-04	0.7076E-05	0.2042E-04	0.2231E-04	0.8195E-05
238.0	1.	0.1000E 06	0.2682E-02	0.2659E-02	0.2923E-02	0.3228E-02	0.3206E-02	0.3340E-02	0.3556E-02	0.3517E-02	0.3558E-02
238.0	1.	0.6000E 05	0.963E-03	0.9462E-03	0.9680E-03	0.1224E-02	0.1208E-02	0.1134E-02	0.1390E-02	0.1370E-02	0.1222E-02
238.0	1.	0.2000E 05	0.1305E-03	0.1285E-03	0.9101E-04	0.2044E-03	0.2057E-03	0.1087E-03	0.3138E-03	0.3428E-03	0.1259E-03
238.0	2.	0.1000E 06	0.2381E-03	0.2354E-03	0.2178E-03	0.3149E-03	0.3103E-03	0.2559E-03	0.3652E-03	0.3595E-03	0.2767E-03
238.0	2.	0.6000E 05	0.9606E-04	0.9460E-04	0.7484E-04	0.1467E-03	0.1448E-03	0.9131E-04	0.1876E-03	0.1874E-03	0.1006E-03
238.0	2.	0.2000E 05	0.2858E-04	0.3893E-04	0.7876E-05	0.9655E-04	0.4576E-04	0.1010E-04	0.3088E-03	0.1918E-04	0.1253E-04
238.0	3.	0.1000E 06	0.6234E-04	0.6144E-04	0.4848E-04	0.9163E-04	0.9023E-04	0.5823E-04	0.1142E-03	0.1130E-03	0.6373E-04
238.0	3.	0.6000E 05	0.2916E-04	0.2878E-04	0.1715E-04	0.5745E-04	0.6176E-04	0.2167E-04	0.8855E-04	0.1213E-03	0.2435E-04
238.0	3.	0.2000E 05	0.2793E-04	0.6151E-05	0.1995E-05	0.2029E-03	0.2506E-05	0.2739E-05	0.9694E-03	0.1797E-05	0.3633E-05
									$P_{FUEL} / P = 0.1$		
1.0	1.	0.1000E 06	0.1748E-03	0.1734E-03	0.1910E-03	0.2112E-03	0.2091E-03	0.2184E-03	0.2320E-03	0.2294E-03	0.2328E-03
1.0	1.	0.6000E 05	0.6237E-04	0.6172E-04	0.6333E-04	0.7988E-04	0.7883E-04	0.7422E-04	0.9075E-04	0.8945E-04	0.8030E-04
1.0	1.	0.2000E 05	0.8494E-05	0.8362E-05	0.5929E-05	0.1414E-04	0.1429E-04	0.7249E-05	0.2047E-04	0.2237E-04	0.8201E-05
238.0	1.	0.1000E 06	0.2686E-02	0.2664E-02	0.2936E-02	0.3244E-02	0.3213E-02	0.3357E-02	0.3564E-02	0.3525E-02	0.3577E-02
238.0	1.	0.6000E 05	0.984E-03	0.9484E-03	0.9731E-03	0.1227E-02	0.1211E-02	0.1143E-02	0.1395E-02	0.1374E-02	0.1229E-02
238.0	1.	0.2000E 05	0.1305E-03	0.1285E-03	0.9111E-04	0.2175E-03	0.2195E-03	0.1114E-03	0.3145E-03	0.3438E-03	0.1263E-03
238.0	2.	0.1000E 06	0.2387E-03	0.2360E-03	0.2190E-03	0.3158E-03	0.3113E-03	0.2575E-03	0.3666E-03	0.3609E-03	0.2786E-03
238.0	2.	0.6000E 05	0.6641E-04	0.6494E-04	0.7532E-04	0.1475E-03	0.1566E-03	0.9199E-04	0.1888E-03	0.1886E-03	0.1016E-03
238.0	2.	0.2000E 05	0.2857E-04	0.3890E-04	0.7888E-05	0.1138E-03	0.3557E-04	0.1046E-04	0.3105E-03	0.1913E-04	0.1254E-04
238.0	3.	0.1000E 06	0.6255E-04	0.6165E-04	0.4877E-04	0.9207E-04	0.9067E-04	0.2865E-04	0.1149E-03	0.1137E-03	0.6424E-04
238.0	3.	0.6000E 05	0.2916E-04	0.2894E-04	0.1728E-04	0.5792E-04	0.6247E-04	0.2166E-04	0.8951E-04	0.1239E-03	0.2458E-04
238.0	3.	0.2000E 05	0.2793E-04	0.6156E-05	0.1999E-05	0.2577E-03	0.2559E-05	0.2865E-05	0.9763E-03	0.1795E-05	0.3639E-05

TABLE IV (CONT'D)

VISCOSITIES OF H^+ , U^+ , U^{++} , AND U^{+++} IONS
 CALCULATED BY THREE DIFFERENT PROCEDURES
 VISCOSITY IN LB/(FT- SEC)

M	Z	T - DEG K	P = 100 ATM			P = 500 ATM			P = 1000 ATM		
			η_L	η_{SC}	η_R	η_L	η_{SC}	η_R	η_L	η_{SC}	η_R
$P_{FUEL} / P = 0.233$											
1.0	1.	0.1000E 06	0.1787E-03	0.1771E-03	0.1997E-03	0.2166E-03	0.2146E-03	0.2298E-03	0.2361E-03	0.2457E-03	0.2387E-03
1.0	1.	0.6000E 05	0.6409E-04	0.6340E-04	0.6667E-04	0.8249E-04	0.8139E-04	0.7847E-04	0.9250E-04	0.8455E-04	0.9388E-04
1.0	1.	0.2000E 05	0.871CE-05	0.8579E-05	0.6019E-05	0.1471E-04	0.1493E-04	0.7353E-05	0.2327E-04	0.8277E-05	0.2107E-04
238.0	1.	0.1000E 06	0.2745E-02	0.2722E-02	0.3068E-02	0.3331E-02	0.3297E-02	0.3530E-02	0.3668E-02	0.3775E-02	0.2387E-03
238.0	1.	0.6000E 05	0.9849E-03	0.9743E-03	0.1024E-02	0.1268E-02	0.1251E-02	0.1206E-02	0.1421E-02	0.1299E-02	0.1443E-02
238.0	1.	0.2000E 05	0.1338E-03	0.1318E-03	0.9248E-04	0.2260E-03	0.2294E-03	0.1130E-03	0.3576E-03	0.1272E-03	0.3238E-03
238.0	2.	0.1000E 06	0.2462E-03	0.2433E-03	0.2308E-03	0.3291E-03	0.3242E-03	0.2740E-03	0.3783E-03	0.2979E-03	0.3844E-03
238.0	2.	0.6000E 05	0.1007E-03	0.9916E-04	0.8029E-04	0.1562E-03	0.159E-03	0.9885E-04	0.2038E-03	0.1091E-03	0.2023E-03
238.0	2.	0.2000E 05	0.3045E-04	0.4428E-04	0.8051E-05	0.1262E-03	0.3441E-04	0.1068E-04	0.3350E-03	0.1650E-04	0.1272E-03
238.0	3.	0.1000E 06	0.6518E-04	0.6421E-04	0.5177E-04	0.9773E-04	0.9632E-04	0.6302E-04	0.1235E-03	0.1227E-03	0.6950E-04
238.0	3.	0.6000E 05	0.3132E-04	0.3098E-04	0.1862E-04	0.6430E-04	0.7188E-04	0.2383E-04	0.1015E-03	0.1632E-03	0.2686E-04
238.0	3.	0.2000E 05	0.3129E-04	0.5609E-05	0.2051E-05	0.2999E-03	0.2274E-05	0.2944E-05	0.1073E-02	0.1766E-05	0.3706E-05
$P_{FUEL} / P = 0.367$											
1.0	1.	0.1000E 06	0.1820E-03	0.1804E-03	0.2056E-03	0.2217E-03	0.2194E-03	0.2377E-03	0.2447E-03	0.2419E-03	0.2547E-03
1.0	1.	0.6000E 05	0.6559E-04	0.6486E-04	0.6897E-04	0.9469E-04	0.8353E-04	0.8130E-04	0.9646E-04	0.9502E-04	0.8752E-04
1.0	1.	0.2000E 05	0.8895E-05	0.8762E-05	0.6080E-05	0.1524E-04	0.1555E-04	0.7446E-05	0.2167E-04	0.2420E-04	0.8350E-05
238.0	1.	0.1000E 06	0.2797E-02	0.2773E-02	0.3160E-02	0.3407E-02	0.3372E-02	0.3652E-02	0.3760E-02	0.3717E-02	0.3914E-02
238.0	1.	0.6000E 05	0.1008E-02	0.9967E-03	0.1060E-02	0.1301E-02	0.1284E-02	0.1249E-02	0.1482E-02	0.1460E-02	0.1345E-02
238.0	1.	0.2000E 05	0.1367E-03	0.1346E-03	0.9342E-04	0.2341E-03	0.2389E-03	0.1144E-03	0.3330E-03	0.3718E-03	0.1283E-03
238.0	2.	0.1000E 06	0.2529E-03	0.2498E-03	0.2392E-03	0.3410E-03	0.3358E-03	0.2858E-03	0.4006E-03	0.3942E-03	0.3119E-03
238.0	2.	0.6000E 05	0.1046E-03	0.1029E-03	0.8379E-04	0.1647E-03	0.1632E-03	0.1035E-03	0.2140E-03	0.2165E-03	0.1142E-03
238.0	2.	0.2000E 05	0.3213E-04	0.4993E-04	0.8163E-05	0.1400E-03	0.3142E-04	0.1087E-04	0.3603E-03	0.1793E-04	0.1288E-04
238.0	3.	0.1000E 06	0.6755E-04	0.6652E-04	0.5390E-04	0.1030E-03	0.1016E-03	0.6619E-04	0.1317E-03	0.1315E-03	0.7335E-04
238.0	3.	0.6000E 05	0.3316E-04	0.3289E-04	0.1957E-04	0.7020E-04	0.8164E-04	0.2521E-04	0.1125E-03	0.2166E-03	0.2843E-04
238.0	3.	0.2000E 05	0.3443E-04	0.5230E-05	0.2087E-05	0.3439E-03	0.2204E-05	0.3014E-05	0.1174E-02	0.1739E-05	0.3771E-05

TABLE IV (CONT'D)
 VISCOSITIES OF H⁺, U⁺, U⁺⁺, AND U⁺⁺⁺ IONS
 CALCULATED BY THREE DIFFERENT PROCEDURES
 VISCOSITY IN LB/(FT-SEC)

M	Z	T-DEG K	P = 100 ATM			P = 500 ATM			P = 1000 ATM			
			η_L	η_{SC}	η_R	η_L	η_{SC}	η_R	η_L	η_{SC}	η_R	
P _{FUEL} / P = 0.5												
1.0	1.	0.1000E 06	0.1849E-03	0.1833E-03	0.2102E-03	0.2261E-03	0.2237E-03	0.2438E-03	0.2471E-03	0.2618E-03	0.2618E-03	
1.0	1.	0.6000E 05	0.6689E-04	0.6614E-04	0.7074E-04	0.8657E-04	0.8531E-04	0.8341E-04	0.9866E-04	0.9717E-04	0.8912E-04	0.8912E-04
1.0	1.	0.2000E 05	0.9059E-05	0.8926E-05	0.6129E-05	0.1573E-04	0.1613E-04	0.7528E-05	0.2223E-04	0.2508E-04	0.8415E-05	0.8415E-05
238.0	1.	0.1000E 06	0.2842E-02	0.2817E-02	0.3223E-02	0.3474E-02	0.3437E-02	0.3746E-02	0.3842E-02	0.3797E-02	0.4022E-02	0.4022E-02
238.0	1.	0.6000E 05	0.1028E-02	0.1016E-02	0.1087E-02	0.1330E-02	0.1312E-02	0.1282E-02	0.1516E-02	0.1493E-02	0.1379E-02	0.1379E-02
238.0	1.	0.2000E 05	0.1392E-03	0.1371E-03	0.9418E-04	0.2417E-03	0.2479E-03	0.1157E-03	0.3416E-03	0.3553E-03	0.1293E-03	0.1293E-03
238.0	2.	0.1000E 06	0.2588E-03	0.2556E-03	0.2457E-03	0.3518E-03	0.3464E-03	0.2951E-03	0.4154E-03	0.4088E-03	0.3229E-03	0.3229E-03
238.0	2.	0.6000E 05	0.1080E-03	0.1063E-03	0.8651E-04	0.1719E-03	0.1707E-03	0.1071E-03	0.2244E-03	0.2285E-03	0.1181E-03	0.1181E-03
238.0	2.	0.2000E 05	0.3368E-04	0.5601E-04	0.8254E-05	0.1529E-03	0.2919E-04	0.1105E-04	0.3844E-03	0.1746E-04	0.1303E-04	0.1303E-04
238.0	3.	0.1000E 06	0.6970E-04	0.6863E-04	0.5558E-04	0.1075E-03	0.1066E-03	C-6871E-04	0.1395E-03	0.1399E-03	0.7643E-04	0.7643E-04
238.0	3.	0.6000E 05	0.3487E-04	0.3467E-04	0.2033E-04	0.7569E-04	0.9183E-04	0.2628E-04	0.1228E-03	0.2511E-03	0.2964E-04	0.2964E-04
238.0	3.	0.2000E 05	0.3740E-04	0.4945E-05	0.2116E-05	0.3883E-03	0.2146E-05	0.3079E-05	0.1270E-02	0.1176E-05	0.3830E-05	0.3830E-05
P _{FUEL} / P = 0.633												
1.0	1.	0.1000E 06	0.1876E-03	0.1859E-03	0.2140E-03	0.2301E-03	0.2276E-03	0.2489E-03	0.2548E-03	0.2518E-03	0.2676E-03	0.2676E-03
1.0	1.	0.6000E 05	0.6806E-04	0.6729E-04	0.7218E-04	0.6824E-04	0.8700E-04	0.8511E-04	0.1006E-03	0.9099E-04	0.9150E-04	0.9150E-04
1.0	1.	0.2000E 05	0.9204E-05	0.9071E-05	0.6170E-05	0.1620E-04	0.1669E-04	0.7603E-05	0.2288E-04	0.2611E-04	0.8487E-05	0.8487E-05
238.0	1.	0.1000E 06	0.2883E-02	0.2857E-02	0.3228E-02	0.3535E-02	0.3497E-02	0.3825E-02	0.3916E-02	0.3870E-02	0.4112E-02	0.4112E-02
238.0	1.	0.6000E 05	0.1046E-02	0.1034E-02	0.1109E-02	0.1356E-02	0.1337E-02	0.1308E-02	0.1545E-02	0.1523E-02	0.1406E-02	0.1406E-02
238.0	1.	0.2000E 05	0.1414E-03	0.1394E-03	0.9482E-04	0.2489E-03	0.2565E-03	0.1168E-03	0.3512E-03	0.4012E-03	0.1304E-03	0.1304E-03
238.0	2.	0.1000E 06	0.2643E-03	0.2609E-03	0.2511E-03	0.3618E-03	0.3562E-03	0.3029E-03	0.4292E-03	0.4224E-03	0.3322E-03	0.3322E-03
238.0	2.	0.6000E 05	0.1112E-03	0.1095E-03	0.8877E-04	0.1785E-03	0.1776E-03	0.1100E-03	0.2341E-03	0.2398E-03	0.1213E-03	0.1213E-03
238.0	2.	0.2000E 05	0.2511E-04	0.6258E-04	0.8331E-05	0.1657E-03	0.2746E-04	0.1121E-04	0.4127E-03	0.1697E-04	0.1320E-04	0.1320E-04
238.0	3.	0.1000E 06	0.7169E-04	0.7058E-04	0.5698E-04	0.1126E-03	0.1114E-03	0.7085E-04	0.1470E-03	0.1482E-03	0.7905E-04	0.7905E-04
238.0	3.	0.6000E 05	0.6648E-04	0.3639E-04	0.2095E-04	0.8093E-04	0.1027E-03	0.2715E-04	0.1328E-03	0.4275E-03	0.3063E-04	0.3063E-04
238.0	3.	0.2000E 05	0.4021E-04	0.4724E-05	0.2141E-05	0.3327E-03	0.2097E-05	0.3137E-05	0.1385E-02	0.1692E-05	0.3839E-05	0.3839E-05

TABLE IV (CONT'D)

**VISSCOSITIES OF H⁺, U⁺, U⁺⁺, AND U⁺⁺⁺ IONS
CALCULATED BY THREE DIFFERENT PROCEDURES
VISSCOSITY IN LB/(FT- SEC)**

M	Z	T - DEG K	P = 100 ATM			P = 500 ATM			P = 1000 ATM		
			η_L	η_{SC}	η_R	η_L	η_{SC}	η_R	η_L	η_{SC}	η_R
					$P_{FUEL}/P = 0.767$						
1.0	1.	0.1000E 06	0.1900E-03	0.1883E-03	0.2173E-03	0.2337E-03	0.2312E-03	0.2533E-03	0.2593E-03	0.2562E-03	0.2727E-03
1.0	1.	0.6000E 05	0.6913E-04	0.6833E-04	0.7342E-04	0.8976E-04	0.8848E-04	0.8654E-04	0.1024E-03	0.1008E-03	0.9301E-04
1.0	1.	0.2000E 05	0.9329E-05	0.9197E-05	0.6620E-05	0.1662E-04	0.1721E-04	0.7670E-05	0.2346E-04	0.2713E-04	0.8553E-05
238.0	1.	0.1000E 06	0.2920E-02	0.2894E-02	0.3339E-02	0.3591E-02	0.3552E-02	0.3892E-02	0.3985E-02	0.3937E-02	0.4190E-02
238.0	1.	0.6000E 05	0.1062E-02	0.1050E-02	0.1128E-02	0.1379E-02	0.1360E-02	0.1330E-02	0.1574E-02	0.1550E-02	0.1429E-02
238.0	1.	0.2000E 05	0.1434E-03	0.1413E-03	0.9533E-04	0.2554E-03	0.2644E-03	0.2644E-03	0.3605E-03	0.4168E-03	0.1314E-03
238.0	2.	0.1000E 06	0.2693E-03	0.2659E-03	0.2558E-03	0.3712E-03	0.3654E-03	0.3097E-03	0.4423E-03	0.4354E-03	0.3403E-03
238.0	2.	0.6000E 05	0.1142E-03	0.1124E-03	0.9071E-04	0.1846E-03	0.1842E-03	0.1125E-03	0.2433E-03	0.2508E-03	0.1203E-03
238.0	2.	0.2000E 05	0.3637E-04	0.6937E-04	0.8396E-05	0.1778E-03	0.2611E-04	0.1135E-04	0.4407E-03	0.1655E-04	0.1336E-04
238.0	3.	0.1000E 06	0.7358E-04	0.7242E-04	0.5820E-04	0.1171E-03	0.1160E-03	0.7273E-04	0.1543E-03	0.1566E-03	0.8137E-04
238.0	3.	0.6000E 05	0.3802E-04	0.3895E-04	0.2150E-04	0.8600E-04	0.1147E-03	0.2791E-04	0.1426E-03	0.7081E-03	0.3130E-04
238.0	3.	0.2000E 05	0.4275E-04	0.4555E-05	0.2162E-05	0.4759E-03	0.2055E-05	0.3191E-05	0.1500E-02	0.1671E-05	0.3398E-05
33											
							$P_{FUEL}/P = 0.9$				
238.0	2.	0.1000E 06	0.1923E-03	0.1905E-03	0.2220E-03	0.2371E-03	0.2345E-03	0.2571E-03	0.2634E-03	0.2602E-03	0.2771E-03
238.0	2.	0.6000E 05	0.7011E-04	0.692E-04	0.7448E-04	0.9114E-04	0.8982E-04	0.8777E-04	0.1041E-03	0.1055E-03	0.9421E-04
238.0	2.	0.2000E 05	0.9423E-05	0.9291E-05	0.6231E-05	0.1697E-04	0.1765E-04	0.7724E-05	0.2398E-04	0.2804E-04	0.8609E-05
238.0	1.	0.1000E 06	0.2954E-02	0.2928E-02	0.3382E-02	0.3643E-02	0.3603E-02	0.3951E-02	0.4048E-02	0.3999E-02	0.4258E-02
238.0	1.	0.6000E 05	0.1077E-02	0.1055E-02	0.1144E-02	0.1400E-02	0.1380E-02	0.1349E-02	0.1595E-02	0.1574E-02	0.1449E-02
238.0	1.	0.2000E 05	0.1448E-03	0.1428E-03	0.9575E-04	0.2608E-03	0.2712E-03	0.1187E-03	0.3685E-03	0.4308E-03	0.1323E-03
238.0	2.	0.1000E 06	0.2740E-03	0.2704E-03	0.2599E-03	0.3800E-03	0.3740E-03	0.3157E-03	0.4547E-03	0.4477E-03	0.3475E-03
238.0	2.	0.6000E 05	0.1169E-03	0.1151E-03	0.9244E-04	0.1904E-03	0.1903E-03	0.1147E-03	0.2519E-03	0.2615E-03	0.1264E-03
238.0	2.	0.2000E 05	0.3733E-04	0.7539E-04	0.8444E-05	0.1883E-03	0.2512E-04	0.1147E-04	0.4656E-03	0.1622E-04	0.1349E-04
238.0	3.	0.1000E 06	0.7534E-04	0.7415E-04	0.5928E-04	0.1213E-03	0.1205E-03	0.7440E-04	0.1614E-03	0.1666E-03	0.8344E-04
238.0	3.	0.6000E 05	0.3945E-04	0.3955E-04	0.2198E-04	0.9089E-04	0.1278E-03	0.2857E-04	0.1521E-03	0.1690E-02	0.3226E-04
238.0	3.	0.2000E 05	0.4475E-04	0.4455E-05	0.2178E-05	0.5135E-03	0.2024E-05	0.3234E-05	0.1602E-02	0.1653E-05	0.4011E-05

TABLE IV (CONT'D)

 BINARY INTERIONIC DIFFUSIVITIES CALCULATED USING
 THREE DIFFERENT PROCEDURES
DIFFUSIVITY, D_{ij} , IN FT²/SEC

P = 1000 ATM, T = 100,000 DEG K

M_1	M_2	Z_1	Z_2	P_{FUEL}/P	P_{FUEL}/P	P_{FUEL}/P
1.0	0.0	1	1	0.09	0.1	0.233
238.0	0.0	1	1	D_L	D_{SC}	D_R
238.0	0.0	2	1	0.3128E+01	0.4108E+01	0.3130E+01
238.0	0.0	3	1	0.3127E+01	0.4107E+01	0.3129E+01
238.0	0.0	2	1	0.9441E+00	0.1326E+01	0.8424E+00
238.0	0.0	3	1	0.4775E+00	0.7109E+00	0.3866E+00
238.0	1.0	1	1	0.7311E+01	0.9601E+01	0.7315E+01
238.0	1.0	2	1	0.2207E+01	0.3101E+01	0.1969E+01
238.0	1.0	3	1	0.1116E+01	0.1662E+01	0.9038E+02
238.0	238.0	2	1	0.2027E+02	0.2848E+02	0.1809E+02
238.0	238.0	3	1	0.1025E+02	0.1526E+02	0.8300E+03
238.0	238.0	3	2	0.3351E-03	0.5889E-03	0.2384E-03
				0.367		0.633
1.0	0.0	1	1	D_L	D_{SC}	D_R
238.0	0.0	1	1	0.3285E+01	0.4383E+01	0.3401E+01
238.0	0.0	2	1	0.3284E+01	0.4381E+01	0.3400E+01
238.0	0.0	3	1	0.1002E+01	0.1443E+01	0.9215E+00
238.0	0.0	2	1	0.5109E+00	0.7878E+00	0.4242E+00
238.0	1.0	1	1	0.7677E+01	0.1024E+00	0.7949E+01
238.0	1.0	2	1	0.2342E+01	0.3374E+01	0.2154E+01
238.0	1.0	3	1	0.1119E+01	0.1842E+01	0.9916E+02
238.0	238.0	2	1	0.2151E+02	0.3099E+02	0.1979E+02
238.0	238.0	3	1	0.1097E+02	0.1691E+02	0.9107E+03
238.0	238.0	3	2	0.3660E+03	0.6932E+03	0.2654E+03
				0.767		0.9
1.0	0.0	1	1	D_L	D_{SC}	D_R
238.0	0.0	1	1	0.3454E+01	0.4689E+01	0.3606E+01
238.0	0.0	2	1	0.3453E+01	0.4688E+01	0.3605E+01
238.0	0.0	3	1	0.1055E+01	0.1579E+01	0.9821E+00
238.0	0.0	2	1	0.5484E+00	0.8810E+00	0.4531E+00
238.0	1.0	1	1	0.8073E+01	0.1096E+00	0.8429E+01
238.0	1.0	2	1	0.2491E+01	0.3692E+01	0.2296E+01
238.0	1.0	3	1	0.1282E+01	0.2060E+01	0.1059E+01
238.0	238.0	2	1	0.2287E+02	0.3391E+02	0.2109E+02
238.0	238.0	3	1	0.1177E+02	0.1892E+02	0.9728E+03
238.0	238.0	3	2	0.4021E+03	0.8388E+03	0.2867E+03

TABLE VI
VISCOSITIES OF EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM
VISCOSITY IN LB/(FT - SEC)

T-DEG K	P _{FUEL} /P = 0.09	0.1	0.233	0.367	0.5	0.633	0.767	0.9
0.1000E 06	0.1752E-03	0.1711E-03	0.1404E-03	0.1175E-03	0.1003E-03	0.8567E-04	0.7559E-04	0.6549E-04
0.6000E 05	0.6219E-04	0.6139E-04	0.5252E-04	0.4556E-04	0.4250E-04	0.3903E-04	0.3756E-04	0.3508E-04
0.2000E 05	0.9458E-04	0.9535E-04	0.1061E-03	0.1364E-03	0.1335E-03	0.9948E-04	0.9516E-04	0.9147E-04
P = 100 ATM								
0.1000E 26	0.2078E-03	0.2047E-03	0.1590E-03	0.1428E-03	0.1232E-03	0.108CE-03	0.9562E-03	0.8566E-03
0.6000E 25	0.7992E-04	0.7769E-04	0.7712E-04	0.7513E-04	0.7613E-04	0.7665E-04	0.7746E-04	0.7841E-04
0.2000E 05	0.1054E-03	0.1469E-03	0.1568E-03	0.1542E-03	0.1480E-03	0.1402E-03	0.1314E-03	0.1224E-03
P = 500 ATM								
0.1000E 26	0.2233E-03	0.2270E-03	0.1856E-03	0.1777E-03	0.1621E-03	0.1493E-03	0.1309E-03	0.1193E-03
0.6000E 25	0.9234E-04	0.9272E-04	0.9577E-04	0.1000E-03	0.1028E-03	0.1052E-03	0.1075E-03	0.1096E-03
0.2000E 05	0.1545E-03	0.1573E-03	0.1711E-03	0.1707E-03	0.1660E-03	0.1584E-03	0.1491E-03	0.1386E-03
P = 1000 ATM								
0.1000E 06	0.2270E-03	0.2233E-03	0.1856E-03	0.1777E-03	0.1621E-03	0.1493E-03	0.1309E-03	0.1193E-03
0.6000E 05	0.9234E-04	0.9272E-04	0.9577E-04	0.1000E-03	0.1028E-03	0.1052E-03	0.1075E-03	0.1096E-03
0.2000E 05	0.1545E-03	0.1573E-03	0.1711E-03	0.1707E-03	0.1660E-03	0.1584E-03	0.1491E-03	0.1386E-03

TABLE VII (CONT'D)

COEFFICIENTS OF DIFFUSION IN EQUILIBRIUM MIXTURES
OF HYDROGEN AND URANIUM

COEFFICIENT OF DIFFUSION, D_{ij} , IN FT^2/SEC

$P = 1000 \text{ ATM}, T = 100,000 \text{ DEG K}$

P_{FUEL} / P

M_1	M_2	$Z_1 Z_2$	0.09	0.1	0.233	0.367	0.5	0.633	0.767	0.9
0.0	1.0 -1	1	0.2791E 02	0.3009E 02	0.5348E 02	0.6901E 02	0.8199E 02	0.9164E 02	0.9962E 02	0.1063E 03
0.0	238.0 -1	1	0.1389E-00	0.1470E-00	0.2394E-00	0.3061E-00	0.3563E-00	0.3963E-00	0.4295E-00	0.4574E-00
0.0	238.0 -1	2	0.1276E-00	0.1366E-00	0.2338E-00	0.3020E-00	0.3531E-00	0.3935E-00	0.4270E-00	0.4552E-00
0.0	238.0 -1	3	0.1252E-00	0.1343E-00	0.2326E-00	0.3011E-00	0.3523E-00	0.3929E-00	0.4264E-00	0.4547E-00
0.0	1.0 -1	0	0.2883E 02	0.3104E 02	0.5455E 02	0.7086E 02	0.8301E 02	0.9262E 02	0.1006E 03	0.1072E 03
1.0	0.0 1	-1	0.1103E 04	0.1199E 04	0.2233E 04	0.2954E 04	0.3491E 04	0.3916E 04	0.4267E 04	0.4562E 04
1.0	238.0 1	1	0.2075E-01	0.1975E-01	0.1413E-01	0.1247E-01	0.1173E-01	0.1135E-01	0.1113E-01	0.1101E-01
1.0	238.0 1	2	0.1094E-01	0.1081E-01	0.1029E-01	0.1031E-01	0.1043E-01	0.1057E-01	0.1072E-01	0.1086E-01
1.0	238.0 1	3	0.8859E-02	0.8902E-02	0.9454E-02	0.9839E-02	0.1014E-01	0.1040E-01	0.1062E-01	0.1082E-01
1.0	1.0 1	0	0.1307E 01	0.1367E 01	0.1857E 01	0.2099E 01	0.2254E 01	0.2369E 01	0.2461E 01	0.2538E 01
238.0	0.0 1	-1	0.3168E 03	0.3220E 03	0.3646E 03	0.3868E 03	0.4024E 03	0.4147E 03	0.4252E 03	0.4343E 03
238.0	1.0 1	1	0.1724E-00	0.1752E-00	0.1984E-00	0.2105E-00	0.2190E-00	0.2257E-00	0.2314E-00	0.2363E-00
238.0	238.0 1	2	0.7303E-03	0.7421E-03	0.8404E-03	0.8917E-03	0.9276E-03	0.9560E-03	0.9800E-03	0.1001E-02
238.0	238.0 1	3	0.7303E-03	0.7421E-03	0.8404E-03	0.8917E-03	0.9276E-03	0.9560E-03	0.9800E-03	0.1001E-02
238.0	1.0 1	0	0.1724E-00	0.1752E-00	0.1984E-00	0.2105E-00	0.2190E-00	0.2257E-00	0.2314E-00	0.2363E-00
238.0	0.0 2	-1	0.8963E 02	0.9145E 02	0.1046E 03	0.1113E 03	0.1159E 03	0.1194E 03	0.1223E 03	0.1246E 03
238.0	1.0 2	1	0.4879E-01	0.4977E-01	0.5694E-01	0.6065E-01	0.6319E-01	0.6515E-01	0.6677E-01	0.6813E-01
238.0	238.0 2	1	0.2085E-03	0.2113E-03	0.2470E-03	0.2668E-03	0.2816E-03	0.2942E-03	0.3054E-03	0.3160E-03
238.0	238.0 2	3	0.2066E-03	0.2109E-03	0.2417E-03	0.2578E-03	0.2689E-03	0.2776E-03	0.2849E-03	0.2912E-03
238.0	1.0 2	0	0.4880E-01	0.4978E-01	0.5698E-01	0.6072E-01	0.6329E-01	0.6529E-01	0.6695E-01	0.6835E-01
238.0	0.0 3	-1	0.1183E 02	0.1145E 02	0.8452E 01	0.6413E 01	0.5003E 01	0.3986E 01	0.3231E 01	0.2699E 01
238.0	1.0 3	1	0.8911E-02	0.8926E-02	0.9588E-02	0.1006E-01	0.1046E-01	0.1081E-01	0.1113E-01	0.1144E-01
238.0	238.0 3	1	0.6781E-03	0.6955E-03	0.8152E-03	0.8716E-03	0.9081E-03	0.9354E-03	0.9573E-03	0.9753E-03
238.0	238.0 3	2	0.1979E-03	0.2027E-03	0.2382E-03	0.2558E-03	0.2677E-03	0.2769E-03	0.2845E-03	0.2910E-03
238.0	1.0 3	0	0.6155E-02	0.6018E-02	0.5316E-02	0.5033E-02	0.4902E-02	0.4841E-02	0.4819E-02	0.4829E-02
1.0	0.0 0	-1	0.1210E 04	0.1253E 04	0.1577E 04	0.1707E 04	0.1779E 04	0.1826E 04	0.1861E 04	0.1888E 04
1.0	1.0 0	1	0.6583E 00	0.6818E 00	0.8578E 00	0.9289E 00	0.9681E 00	0.9939E 00	0.1013E 01	0.1028E 01
1.0	238.0 0	1	0.2833E-02	0.2929E-02	0.3650E-02	0.3943E-02	0.4105E-02	0.4212E-02	0.4290E-02	0.4352E-02
1.0	238.0 0	2	0.2804E-02	0.2903E-02	0.3640E-02	0.3938E-02	0.4102E-02	0.4210E-02	0.4290E-02	0.4352E-02
1.0	238.0 0	3	0.2797E-02	0.2896E-02	0.3637E-02	0.3936E-02	0.4102E-02	0.4210E-02	0.4289E-02	0.4352E-02

TABLE VIII
EFFECTIVE BINARY DIFFUSIVITIES
IN EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM

T - DEG K	P _{FUEL} / P = 0.09	0.1	0.233	0.367	0.5	0.633	0.767	0.9
3.1000E 06	0.1667E-00	0.1678E-00	0.2015E-00	0.2595E-00	0.3246E-00	0.3916E-00	0.3289E-00	0.3289E-00
0.6000E 05	0.3323E-01	0.3386E-01	0.4153E-01	0.5451E-01	0.6014E-01	0.6538E-01	0.7021E-01	0.7021E-01
0.2000E 05	0.1030E-01	0.1026E-01	0.1375E-01	0.1488E-01	0.1038E-01	0.1038E-01	0.1038E-01	0.1038E-01
3.1000E 06	0.3755E-01	0.3802E-01	0.4625E-01	0.6101E-01	0.6699E-01	0.1622E-01	0.6686E-01	0.6686E-01
2.6000E 05	0.879E-02	0.8441E-02	0.1072E-01	0.1268E-01	0.1442E-01	0.1744E-01	0.1877E-01	0.1877E-01
0.2000E 05	0.6119E-02	0.3538E-02	0.4719E-02	0.7795E-02	0.5946E-02	0.2154E-02	0.2154E-02	0.2154E-02

P = 1000 ATM

3.1000E 06	0.1985E-01	0.2024E-01	0.2475E-01	0.2871E-01	0.3228E-01	0.3558E-01	0.3864E-01	0.4132E-01
3.6000E 05	0.4748E-02	0.4834E-02	0.6272E-02	0.7428E-02	0.8431E-02	0.9344E-02	0.1017E-01	0.1087E-01
3.2000E 05	0.1753E-02	0.1792E-02	0.2565E-02	0.3203E-02	0.3617E-02	0.3521E-02	0.2288E-02	0.2288E-02

TABLE IX

FLUX CALCULATION COEFFICIENTS
IN EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM

T - DEG K	P _{FUEL} / P = 0.09	0.1	0.233	0.367	0.5	0.633	0.767	0.9
3.1000E 06	0.1899E-25	0.1714E-25	0.7704E-26	0.4955E-26	0.3663E-26	0.2901E-26	0.2400E-26	0.2049E-26
3.6000E 05	0.1891E-25	0.1717E-25	0.7715E-26	0.4962E-26	0.3663E-26	0.2904E-26	0.2402E-26	0.2050E-26
3.2000E 05	0.2534E-25	0.2353E-25	0.1038E-25	0.6574E-26	0.4764E-26	0.3682E-26	0.2931E-26	0.2338E-26

3.1000E 06	0.1889E-25	0.1717E-25	0.7709E-26	0.4958E-26	0.3661E-26	0.2902E-26	0.2401E-26	0.2049E-26
0.6000E 05	0.1898E-25	0.1724E-25	0.7733E-26	0.4977E-26	0.3673E-26	0.2910E-26	0.2405E-26	0.2051E-26
0.2000E 05	0.1015E-24	0.2534E-25	0.1135E-25	0.7292E-26	0.5351E-26	0.4177F-26	0.3352E-26	0.2672E-26

3.1000E 06	0.1890E-25	0.1719E-25	0.7711E-26	0.4960E-26	0.3663E-26	0.2903E-26	0.2401E-26	0.2050E-26
0.6000E 05	0.1905E-25	0.1730E-25	0.7663E-26	0.4988E-26	0.3680E-26	0.2914E-26	0.2408E-26	0.2053E-26
0.2000E 05	0.2757E-25	0.2507E-25	0.1144E-25	0.7464E-26	0.5548E-26	0.4177F-26	0.3352E-26	0.2672E-26

TABLE X
EFFECTIVE MASS OF URANIUM SPECIES
IN EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM

T-DEG K	P _{FUEL} /P = 0.09	O.1	O.233	0.367	0.5	0.633	0.767
0.1000E 06	0.2178E-24	0.2178E-24	0.2179E-24	0.2179E-24	0.2179E-24	0.2179E-24	0.2180E-24
0.6000E 05	0.2189E-24	0.2190E-24	0.2205E-24	0.2222E-24	0.2236E-24	0.225CE-24	0.2276E-24
0.2000E 05	0.3730E-24	0.3874E-24	0.4091E-24	0.4172E-24	0.4215E-24	0.4241E-24	0.4272E-24

P = 100 ATM							
0.1000E 06	0.2178E-24	0.2180E-24	0.2182E-24	0.2183E-24	0.2185E-24	0.2186E-24	0.2187E-24
0.6000E 05	0.2230E-24	0.2236E-24	0.2302E-24	0.2353E-24	0.2398E-24	0.2435E-24	0.2469E-24
0.2000E 05	0.3842E-24	0.4215E-24	0.4293E-24	0.4312E-24	0.4323E-24	0.4329E-24	0.4334E-24

P = 500 ATM							
0.1000E 06	0.2179E-24	0.2179E-24	0.2182E-24	0.2183E-24	0.2185E-24	0.2186E-24	0.2187E-24
0.6000E 05	0.2276E-24	0.2286E-24	0.2387E-24	0.2461E-24	0.2517E-24	0.2562E-24	0.2631E-24
0.2000E 05	0.4272E-24	0.4280E-24	0.4321E-24	0.4333E-24	0.4338E-24	0.4344E-24	0.4345E-24

TABLE XI
EFFECTIVE MASS OF HYDROGEN SPECIES
IN EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM

T-DEG K	P _{FUEL} /P = 0.09	O.1	O.233	0.367	0.5	0.633	0.767
0.1000E 06	0.1853E-26	0.1846E-26	0.1845E-26	0.1846E-26	0.1846E-26	0.1846E-26	0.1846E-26
0.6000E 05	0.1849E-26	0.1849E-26	0.1848E-26	0.1848E-26	0.1848E-26	0.1847E-26	0.1847E-26
0.2000E 05	0.2487E-26	0.2488E-26	0.2461E-26	0.2427E-26	0.2384E-26	0.2327E-26	0.2244E-26

P = 1000 ATM							
0.1000E 06	0.1848E-26	0.1848E-26	0.1847E-26	0.1847E-26	0.1847E-26	0.1847E-26	0.1847E-26
0.6000E 05	0.1854E-26	0.1854E-26	0.1853E-26	0.1852E-26	0.1851E-26	0.1849E-26	0.1848E-26
0.2000E 05	0.2586E-26	0.2590E-26	0.2652E-26	0.2641E-26	0.2623E-26	0.2591E-26	0.2529E-26

T-DEG K	P _{FUEL} /P = 0.09	O.1	O.233	0.367	0.5	0.633	0.767
0.1000E 06	0.1848E-26	0.1848E-26	0.1847E-26	0.1847E-26	0.1847E-26	0.1847E-26	0.1847E-26
0.6000E 05	0.1858E-26	0.1858E-26	0.1857E-26	0.1854E-26	0.1853E-26	0.1851E-26	0.1849E-26
0.2000E 05	0.2586E-26	0.2590E-26	0.2617E-26	0.2638E-26	0.2650E-26	0.2650E-26	0.2650E-26

TABLE XIII
EFFECTIVE BINARY SCHMIDT NUMBERS
IN EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM

T - DEG K	P _{FUEL} /P = 0.09	0.1	0.233	0.367	0.5	0.633	0.767	0.9
0.1000E 06	0.2372E-00	0.2090E-00	0.6415E-01	0.3000E-01	0.1691E-01	0.1056E-01	0.7047E-02	0.4948E-02
0.6000E 05	0.2524E-00	0.2218E-00	0.6909E-01	0.3359E-01	0.1994E-01	0.1328E-01	0.9517E-02	0.7226E-02
0.2000E 05	0.2398E-00	0.2206E-00	0.7664E-01	0.4425E-01	0.2189E-01	0.3466E-01		

P = 100 ATM								
0.1000E 06	0.2498E-00	0.2217E-00	0.6727E-01	0.3156E-01	0.1791E-01	0.1131E-01	0.7639E-02	0.5637E-02
0.6000E 05	0.2554E-00	0.2266E-00	0.7539E-01	0.3955E-01	0.2521E-01	0.1786E-01	0.1356E-01	0.1071E-01
0.2000E 05	0.3552E-00	0.1810E-00	0.6418E-01	0.2471E-01	0.2319E-01		0.3808E-01	
P = 500 ATM								
0.1000E 06	0.2581E-00	0.2262E-00	0.6899E-01	0.3253E-01	0.1858E-01	0.1192E-01	0.8068E-02	0.5842E-02
0.6000E 05	0.2529E-00	0.2255E-00	0.7803E-01	0.4244E-01	0.2773E-01	0.1996E-01	0.1526E-01	0.1227E-01
0.2000E 05	0.2114E-00	0.1908E-00	0.6553E-01	0.3432E-01	0.2229E-01	0.1769E-01	0.2162E-01	

P = 1000 ATM								
0.1000E 06	0.2581E-00	0.2262E-00	0.6899E-01	0.3253E-01	0.1858E-01	0.1192E-01	0.8068E-02	0.5842E-02
0.6000E 05	0.2529E-00	0.2255E-00	0.7803E-01	0.4244E-01	0.2773E-01	0.1996E-01	0.1526E-01	0.1227E-01
0.2000E 05	0.2114E-00	0.1908E-00	0.6553E-01	0.3432E-01	0.2229E-01	0.1769E-01	0.2162E-01	
P = 5000 ATM								
0.1000E 06	0.2961E 00	0.2746E 01	0.1265E 01	0.8519E 00	0.6430E 00	0.5190E 00	0.4356E 00	0.3767E 00
0.6000E 05	0.6020E 00	0.5498E 00	0.2617E 00	0.7522E 00	0.1337E 00	0.1088E 00	0.9214E 00	0.8033E 00
0.2000E 05	0.1416E 00	0.1285E 00	0.7100E 01	0.5005E 01	0.3403E 01	0.1977E 01		

P = 10000 ATM								
0.1000E 06	0.6847E 00	0.6221E 00	0.2951E 00	0.1964E 00	0.1489E 00	0.1205E 00	0.1014E 00	0.8804E 00
0.6000E 05	0.1465E 00	0.1338E 00	0.6533E 01	0.4457E 01	0.3450E 01	0.2846E 01	0.2439E 01	0.2147E 01
0.2000E 05	0.2065E 00	0.4426E 00	0.2541E 01	0.2355E 01	0.1413E 01	0.3791E 02		
P = 100000 ATM								
0.1000E 06	0.3629E 00	0.3314E 00	0.1577E 00	0.1052E 00	0.7989E 01	0.6482E 01	0.5470E 01	0.4735E 01
0.6000E 05	0.8207E 01	0.7498E 01	0.3719E 01	0.2557E 01	0.1990E 01	0.1649E 01	0.1418E 01	0.1246E 01
0.2000E 05	0.2499E 01	0.2324E 01	0.1397E 01	0.1068E 01	0.8569E 02	0.6555E 02	0.3800E 02	

**LIST OF PROGRAM SOURCE DECK FOR CALCULATING ELECTRONIC ENERGIES
BY THE METHOD OF LAYER (REF. 9)**

```

250 XAP(111) = 1.000
C STATEMENTS 27 THRU 33 EVALUATE PIAA
C
27 PIAA = 0.000
29 KUP = 2*41 - 1
DO 30 K = 1, KUP + 2
KR = K-1
TP(KR) = 31.31-32
31 PIAA = PIAA + FPART(INA,NA,KR+1,1)
GO TO 30
32 PIAA = PIAA - 5D0*(12.000*P1-1.000)/(4.000*P1-3.000) +
CUM(LL1,L1,K) * FPART(INA,NA,KR+1,1)
30 CONTINUE
33 PIAA = 4.000 + PIAA
34 CONTINUE
C
35 SUM = 0.000
36 DO 50 J = 1, NELC
PIAB = 0.000
IF(J=J) 35,30,35
35 NB = IND(J)
ORJ = NMODX(J)
DO 25 JJ = 1,20
LJ = IND(J) - 20*JJ + 1
PJ = LJ
IF(LJ = 19) 26,26,25
25 CONTINUE
26 NJ = JJ
XAP(1) = 1.000
XAP(2) = 2*LIST(12+1)/2*LIST(12+J)
DO 251 LL = 3, 60
251 XAP(LL) = XAP(2)*XAP(LL-1)
C STATEMENTS 36 THRU 38 EVALUATE PIAB
36 PIAB = PIAB + FPART(INA,NB,0,1,J)
KUP = LI + LJ - 1
DO 37 K = 1, KUP
KR = K - 1
IF(MOD((LI+J)+K-3),2) 37,137,37
37 CONTINUE
PIAB = PIAB - 2500 * CURN(LI,L,J,K) * GPART(INA,NB,KR,1,J)
38 PIAB = 4.000 + PIAB
40 WRITE (6,61) J, 17, PIAB
40 WRITE (6,61) (6,61) J, 17, PIAB
41 WRITE (6,61) (6,61) J, 17, PIAB
40 WRITE (6,61) (6,61) J, 17, PIAB
41 WRITE (6,61) (6,61) J, 17, PIAB
50 SUM = SUM + ONJPIAB
PI(12+1) = SUM + (ON1 - 1.CD0) * PIAB
51 CONTINUE
1F(12-22) = 77.68,77
68 12 = NO2S
69 GO TO 28
77 DO 71 1=1,NELC
NA = IND(K1)
DO 72 11 = 1,20
L1 = NA - 20*11 + 1
IF(L1 = 19) 73,73,72
72 CONTINUE
73 NI = 11
FNI = NI
ZOL(12+1) = 2*LIST(12+1)

71 ZL1ST(12+1) = 2.000 + (20 + DELZ(12)) /FNI - PI(12+1)
WRITE (6,95) 12,ZL1ST(12+1), 1=1,NELC
PRINT 95, 12, (ZL1ST(12+1), 1=1,NELC)
12A = 20 + DELZ(12)
ENER = 0.000
DO 170 MN = 1,NELC
PMEL = NINDX(MN)
170 ENER = ENER - 1.2500 * PMEL*ZL1ST(12,MN)*ZL1ST(12,MN)
WRITE (6,151) 12A,ENER
95 FORMAT (3X,SHZL1ST(5X,4HZ) = 12/de20.8)
C TEST FOR CONVERGENCE
C
1SPY = 0
62 DO 125 I = 1,NELC
ZTEST = ZL1ST(12+1) - ZOLD(12+1)
124 IAMS = (ZTEST) - EPS1 124,124,123
123 AGAIN(I) = 1.0
1SPY = 1
GO TO 125
124 AGAIN(I) = 0.0
125 CONTINUE
1F(1SPY) 126,163,126
126 ICOUNT = 126,163,126
1F(1C0UT-ICOUNT) 167, 187, 20
83 CONTINUE
1F(12+1) 67,67,165
65 IF(1DH) 167,166,167
166 IF(1HP) 165,165,165
165 12,12,-1
167 GO TO 28
C OPTIMIZING OF SCREENING PARAMETERS COMPLETED
C
167 WRITE (6,9)
1SP = (N025 + 2) / 3
DO 78 I = 1, 1UP
I1 = NO25 + 1 - 1
1B = 1A - 1UP
I1 = IB - 1UP
12A = 20 + DELZ(1A)
12B = 20 + DELZ(1B)
12C = 20 + DELZ(1C)
1F (1C) 274,174,741
741 WRITE (6,11) 12A,12B
DO 74 J = 1,NELC
740 WRITE (6,8) IND(J),ZL1ST(1A,J),INDX(J),ZL1ST(1B,J)
1C(J)
74 GO TO 78
174 WRITE (6,11) 12A,12B
DO 175 J = 1,NELC
175 WRITE (6,4) IND(J),ZL1ST(1A,J),INDX(J),ZL1ST(1B,J)
GO TO 75
274 WRITE (6,11) 12A
DO 275 J = 1,NELC
275 WRITE (6,5) IND(J),ZL1ST(1Z,J)
75 CONTINUE
C ENERGY CALCULATION
C

```

**LIST OF PROGRAM SOURCE DECK FOR CALCULATING ELECTRONIC ENERGIES
BY THE METHOD OF LAYZER (REF. 9)**

```

184 DO 80 I = 1,N025
185 T2A = 20 + DEL2(I)
ENER = 0.000
DO 85 J = 1,NELC
FN = NINDX(J)
85 ENER = ENER - 12500 * FN * ZL1ST(1,J)**2
      WRITE(6,15) T2A,ENER
80 CONTINUE
GO TO 187
185 ENER = 0.000
DO 186 J = 1,NELC
FN = NINDX(J)
186 ENER = ENER - 12500 * FN * ZL1ST(12,J)**2
      WRITE(6,15) T2A,ENER
187 IF (IMDA1) 90,90,118
90 CALL EXIT
STOP
END

$18PTC FPART LIST,M04/2
C FPART
C COMPUTES PARTIAL DERIVATIVES OF SLATER 2 ELECTRON P-FUNCTION WRT 2
C PROGRAMMED FROM ANALYSIS DATED 1/26/65
C
C DOUBLE PRECISION FUNCTION FPART(N1,N2,PK,11,12)
C           FACT(40), QL1ST(10,10), DL1ST(12,10,10),
C           ALIST(20,10,10)
C           DIMENSION DL1ST(22,10,10), Nindx(30), XAP(60),
C           TWO(45)
C COMMON FACT, QL1ST, DL1ST, XAP, TWO
C DOUBLE PRECISION FACT, QL1ST, DL1ST, ALIST, XAP, TWO
C DOUBLE PRECISION F2, FN9, FN8, ACDEF, .
C DOUBLE PRECISION ACDE, FN9X, FB90, FDUR, SUM, PNJR
C K = PK
PK=K
DO 1 N=1,20
LA=N-20*NA+1
LA2 = LA+LA
IF(LA-20) 2,2,1
1 CONTINUE
2 NA=NA
DO 3 NB=1,20
LB=NB-20*NB+1
LB2 = LB+LB
TF (LB-20) 4, 4, 3
3 CONTINUE
4 NB=NB-1
F1 = -PK * CAPA(K,NA,LA) + CAPA(-K-1,NA,LB) / XAP(K+2)
FBUP = NA+NA-LA-LB+1
F2 = 0.000
DO 10 IP = 1,IPUP
IPR = IP-1
NP4 = LA2+K+IP
NP6 = LA2-K-1+IP
ACOF = AL1ST(IP,NA,LA)
DO 10 I = 1,IPUP
T0I = 10-
ACOF = ACOF*AL1ST(10,NA,LB)
NP9 = LB+10*
PN9 = NP9
PN9X = PN9*XAB(12)
IPUP = LA2+K-1+IP
DO 10 I = 1,IPUP
NP8 = LA2+IPR-1
NP3 = LB2+IPR+NP8
NP5 = NP8-1
NP7 = NP8-1
NP8 = NP8
PN9 = (PN9-(PN9X))/ACDEF
JUP = (IPUP+1)*UP-10*I+1
NP1 = JUP
DO 10 J = 1,JPUP
JRA-J-1
NP2 = JUP-JR
NP10 = (FACT(NP1)/FACT(NP21)*(FACT(NP2)/FACT(NP3))/FACT(1,J))
NP10 = NP8-1+JR
IF (K+1-NP8) 7,7,8
7 B = FACT(NP1)/FACT(NP2) - FACT(NP6)/FACT(NP7)
GO TO 12
8 B = FACT(NP1)/FACT(NP5),
12 IP = (IP10 - 1) 10, 15
16 NP10 = -NP10+1
F2 = F2 + B*PN9*FB90 / XAP(NP10)
GO TO 10
15 F2 = F2 + B*FDUR*FB90 * XAP(NP10+1)
10 CONTINUE
13 FPART = (QL1ST(NA,LA) * QL1ST(NB,LB))**2 +
      XAP(21) * 2*NA + 2*NB+1) * F2)
      RETURN
END

$18PTC GPART LIST,M04/2
C GPART
C PROGRAMMED FROM ANALYSIS DATED 1/26/65
C DOUBLE PRECISION FACT, QL1ST, DL1ST, XAP, TWO
C           COFF, FN97, TERM
C           FACT(40), QL1ST(10,10,10), DL1ST(12,10,10),
C           ALIST(20,10,10)
C           DIMENSION DL1ST(22,10,10), Nindx(30), XAP(60),
C           TWO(45)
C COMMON FACT, QL1ST, DL1ST, XAP, TWO
C           COFF, FN97, TERM
C           FACT(40), QL1ST(10,10,10), DL1ST(12,10,10),
C           ALIST(20,10,10)
C           DIMENSION DL1ST(22,10,10), Nindx(30), XAP(60),
C           TWO(45)
C
DO 1 NA=1,20
LA=N-20*NA+1
LA2 = LA+LA
IF(LA-20) 2,2,1
1 CONTINUE
2 NA=NA
DO 3 NB=1,20
LB=NB-20*NB+1
LB2 = LB+LB
TF (LB-20) 4, 4, 3
3 CONTINUE
4 NB=NB-1
F1 = -PK * CAPA(K,NA,LA) + CAPA(-K-1,NA,LB) / XAP(K+2)
FBUP = NA+NA-LA-LB+1
F2 = 0.000
DO 10 IP = 1,IPUP
IPR = IP-1
NP4 = LA2+K+IP
NP6 = LA2-K-1+IP
ACOF = AL1ST(IP,NA,LA)
DO 10 I = 1,IPUP
T0I = 10-
ACOF = ACOF*AL1ST(10,NA,LB)
NP9 = LB+10*
PN9 = NP9
PN9X = PN9*XAB(12)
IPUP = LA2+K-1+IP
DO 10 I = 1,IPUP
NP8 = LA2+IPR-1
NP3 = LB2+IPR+NP8
NP5 = NP8-1
NP7 = NP8-1
NP8 = NP8
PN9 = (PN9-(PN9X))/ACDEF
JUP = (IPUP+1)*UP-10*I+1
NP1 = JUP
DO 10 J = 1,JPUP
JRA-J-1
NP2 = JUP-JR
NP10 = (FACT(NP1)/FACT(NP21)*(FACT(NP2)/FACT(NP3))/FACT(1,J))
NP10 = NP8-1+JR
IF (K+1-NP8) 7,7,8
7 B = FACT(NP1)/FACT(NP2) - FACT(NP6)/FACT(NP7)
GO TO 12
8 B = FACT(NP1)/FACT(NP5),
12 IP = (IP10 - 1) 10, 15
16 NP10 = -NP10+1
F2 = F2 + B*PN9*FB90 / XAP(NP10)
GO TO 10
15 F2 = F2 + B*FDUR*FB90 * XAP(NP10+1)
10 CONTINUE
13 FPART = (QL1ST(NA,LA) * QL1ST(NB,LB))**2 +
      XAP(21) * 2*NA + 2*NB+1) * F2)
      RETURN
END

```

TABLE XIV (CONT'D)

LIST OF PROGRAM SOURCE DECK FOR CALCULATING ELECTRONIC ENERGIES
BY THE METHOD OF LAYER (REF. 9)

```

2 NA=NA
LA=LA
LB= 1.000 + XAP(12)
DO 3 NB=1,20
LB = NB-2+NB+1
IF(LB>20) 4,*+3
3 CONTINUE
4 NB=NB
LB2 = LB-LB
NAST = NA-LA
NAST = NAST + 1
NBSTR = NB-LB
NBSTR = NBSTR +1
G1 = 0.000
KAB = KALAHRA+
DO 10 IP = 1,NAST
IPR = IPI-I
DL1 = DLIST(IP,NA,LA)
DO 10 IO = 1,NBSTR
IO= 10 - 1,NBSTR
DL12 = DLIST(IO,NB,LB)*DL1
LT2 = LA2+LB2+IO*IPR
NP2 = LA1,BK4+IPR+IPR
LIO = LB2+IPR
DL123 = DLIST(11,NA,LA) + DL12
I = 11-1
I = 11-1
DO 10 II = 1,NAST
II = 11-1
II = 1,NAST
NP4 = LA2+IPR+IPR
NP6 = XAP(NP4+1)
NP7 = NP3+1
K1AB = KAB + 1
NP3J = LT2 + 1 + I
DO 10 JJ = 1,NBSTR
JJ = JJ-1
COEF = DLIST(JJ,NP,LB)*DL123
NP1 = K1AB + J
NP3 = NP3J + J
NFS = NP3+1
NP7 = LIO + J
TERM = 0.000
DO 8 MM = 1,NP1
MM = MM-1
NP8 = NP3-MM
NP9 = NP3-MM
TERM = TERM +
T2 = TWO(NP3+1)
T3 = FACT(NP1)*(-TERM + FACT(NP2)*T2)
T4 = FNPF6 - FNPF7*XAP(12)
T61 = T60 ** NFS
T6 = 1.000/T61
T7 = T3 * T4 * T5 * T6
G1 = G1 + COEF * T7
10 CONTINUE
13 GPART = 2.000 + (DLIST(NA,LA) + DLIST(NB,LB))**2 + G1
RETURN
END

S1B7TC ALFA LIST.N94/2
C ALFA
SUBROUTINE ALFA(N,L,ALIST)
C COMPUTES ALPHAP(N,L) FOR HYPERGEOMETRIC FUNCTION SQUARED AND
C STORES THEM IN ALIST(N,L+1)
C DIMENSION FACT(10),DLIST(10,10),DLST(20,10,10).
1 ALIST(1120,10,10) DLST(20,10,10).
COMMON FACT * ALIST * DLIST * ALIST
DOUBLE PRECISION FACT * ALIST * DLIST * ALIST * A
DO 1 IN = 1,N
DO 1 IL = 1,N
DO 1 LL = 1,L
LUP = 1N-IL+
A = 0.000
DO 1 IP = 1,NUP
IP1 = 1I - IP + 1
3 IF(IP1>10) 3,3,1
2 A = DLIST(IP,IN,IL) + DLIST(IP,IN,IL) + A
1 ALIST(1,IN,IL) = A
1 CONTINUE
RETURN

S1B7TC CAPA LIST.N94/2
C CAPA
DOUBLE PRECISION FUNCTION CAPA (K,N,LL)
DIMENSION FACT(40),DLIST(20,10,10),DLST(20,10,10).
1 ALIST(1120,10,10) DLST(20,10,10).
COMMON FACT * ALIST * DLIST * ALIST
DOUBLE PRECISION FACT * ALIST * DLIST * ALIST * A
DOUBLE PRECISION FAC
L = LL
A = 0.000
NSTRN=L
IT1 = L-L+K
DO 11 I = 1,NP
NP1 = IT1+1
IF (NP1>11) 3,3,1
3 FAC = FACT(NP1)
11 A = A + ALIST(1,N,L) * FAC
CAPA = A
RETURN
END

S1B7TC CUMC LIST.N94/2
C CUMC
DOUBLE PRECISION FUNCTION CUMC (L1,L2,M)
DIMENSION FACT(40),DLIST(10,10),DLST(20,10,10).
1 ALIST(1120,10,10) DLST(20,10,10).

```

**LIST OF PROGRAM SOURCE DECK FOR CALCULATING ELECTRONIC ENERGIES
BY THE METHOD OF LAYZER (REF. 9)**

```

COMMON FACT * QLIST * DLIST * ALIST * DLST * ALIST * CVM
DOUBLE PRECISION FACT
K = KK
CVM = 0.000
L12 = L1+L2
IG1 = L12*K-3
IG2 = MOD(IG1,2) 9,1,9
IG = IG1/2
L1K = L12 - K
L2K = L12 + K - L1
IF(L2K .LT. 9,9,2
2 NLL = K * L1 - L2
IF(K.LT.1) 9,9,3
3 IGL = IG + IG + 2
I11 = IG+2
I12 = IG+1
I13 = I11-2
I14 = I11-K
CVM = (2.0*FACT(IG+1)*FACT(I1K)*FACT(I1L)*FACT(I1M)) /
1 (FACT(IG)*FACT(IG2)*FACT(IG3)*2*FACT(IG4)*2)
9 RETURN
END

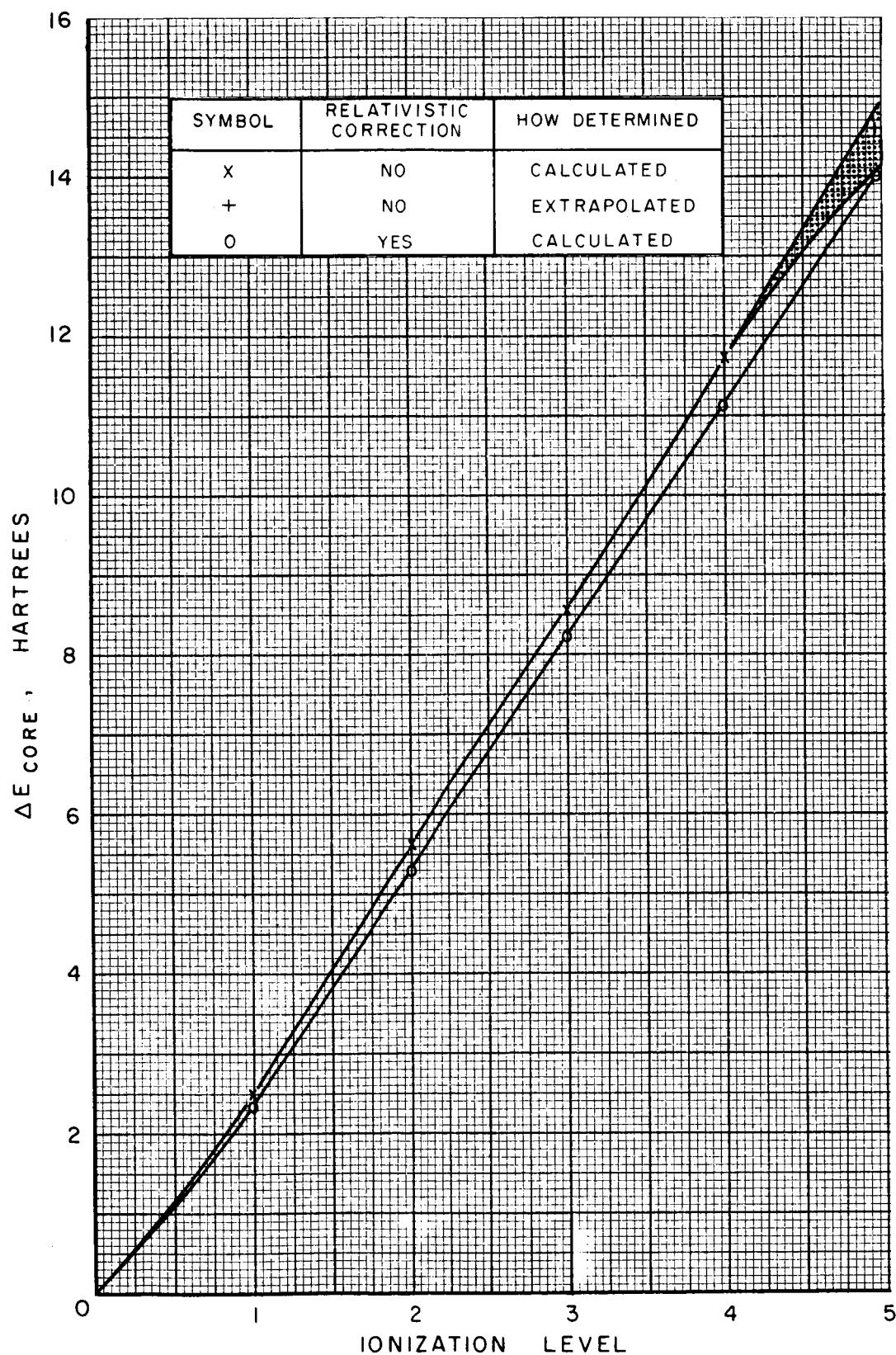
SIBFTC D1NL LIST*.M9A/2
C D1NL
SUBROUTINE D1NL(NL,DL1ST)
C COMPUTES COEFFICIENTS FOR THE HYPERGEOMETRIC FUNCTIONS AND STORES
C THEM IN DL1ST(NL).
C DIMENSION DL1ST(NL),DL1ST(10,10),DL1ST(20,10,10),
1 ALIST(20,10,10)
COMMON FACT * QLIST * DLIST * ALIST * DL1ST * ALIST * D
DOUBLE PRECISION FACT
D = 0.000
DO 1 IN1N
DO 1 IN1L
DO 1 IL=1,IN
1 = IL-1
IUP=IN-1
DO 1 IT=1,IUP
IA = IT-1
NF1 = IN-1
NF2 = NF1-1
NF3 = 1+I+2
NF4 = NF3-1A
D = (-1.0)*I*(FACT(NF1)*FACT(NF2))/FACT(NF3)
1 (FACT(NF4)*FACT(NF5))/FACT(NF6)
1 DL1ST(1,IN,IL) = D
END

SIBFTC FACT LIST*.M9A/2
C FACT
SUBROUTINE FACTX(1,FACT)

```

**VARIATION OF CORE ENERGY WITH IONIZATION LEVEL
FOR THE URANIUM ATOM**

1 HARTREE = 2 • IONIZATION POTENTIAL OF HYDROGEN

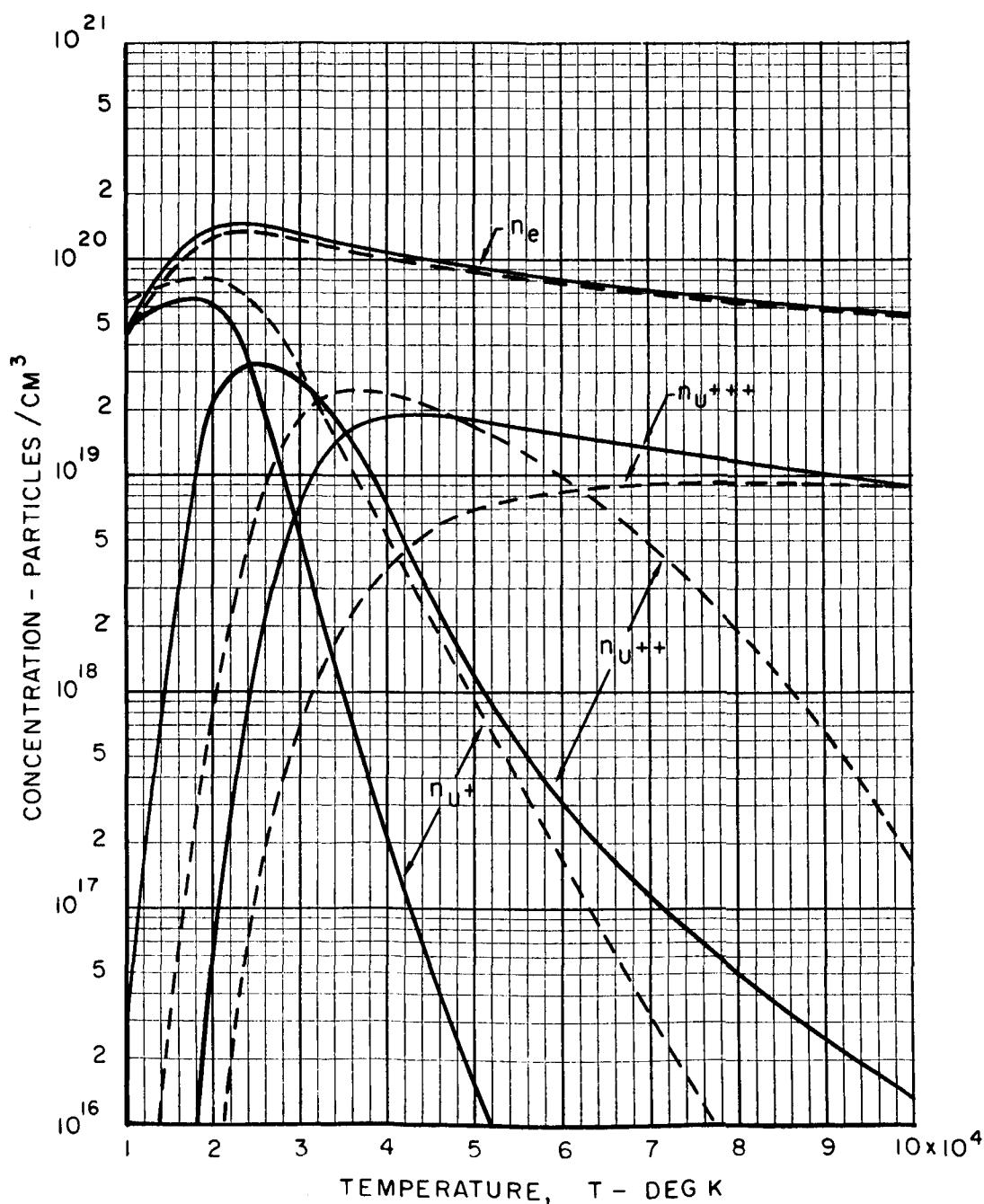


COMPOSITIONS OF EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM USING TWO DIFFERENT SETS OF IONIZATION POTENTIALS FOR URANIUM IONS

$P = 1000 \text{ ATM}$

$P_{\text{FUEL}} / P = 0.5$

— $U(\text{I}) = 6.0 \text{ ev.}, U(\text{II}) = 10.0 \text{ ev.}, U(\text{III}) = 18.0 \text{ ev.}$
 - - - $U(\text{I}) = 6.1 \text{ ev.}, U(\text{II}) = 17.1 \text{ ev.}, U(\text{III}) = 38.8 \text{ ev.}$



**RANGE OF SCHMIDT NUMBERS
IN EQUILIBRIUM MIXTURES OF HYDROGEN AND URANIUM**

